1,2-Cyclohexanedicarboxylic acid, diisobutyl ester

Other names: diisobutyl hexahydrophthalate
Inchi: InChI=1S/C16H28O4/c1-11(2)9-19-15(17)13-7-5-6-8-14(13)16(18)20-10-12(3)4/h11-14H
InchiKey: QUKHPBOCBWDYMW-UHFFFAOYSA-N
Formula: C16H28O4
SMILES: CC(C)COC(=O)C1CCCCC1C(=O)OCC(C)C
Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	-372.14	kJ/mol	Joback Method
hf	-839.75	kJ/mol	Joback Method
hfus	28.63	kJ/mol	Joback Method
hvap	68.87	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.191		Crippen Method
mcvol	240.320	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
rinpol	1845.00		NIST Webbook
rinpol	1845.00		NIST Webbook
tb	732.06	K	Joback Method
tc	933.91	K	Joback Method
tf	387.54	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.85	J/mol×K	900.27	Joback Method
cpg	830.10	J/mol×K	933.91	Joback Method
cpg	732.39	J/mol×K	732.06	Joback Method
cpg	751.74	J/mol×K	765.70	Joback Method
cpg	769.85	J/mol×K	799.34	Joback Method
cpg	786.74	J/mol×K	832.99	Joback Method
cpg	802.40	J/mol×K	866.63	Joback Method

dvisc	0.0001020	Pa×s	732.06	Joback Method
dvisc	0.0001365	Pa×s	674.64	Joback Method
dvisc	0.0021382	Pa×s	387.54	Joback Method
dvisc	0.0009283	Pa×s	444.96	Joback Method
dvisc	0.0004877	Pa×s	502.38	Joback Method
dvisc	0.0002924	Pa×s	559.80	Joback Method
dvisc	0.0001928	Pa×s	617.22	Joback Method
rfi	1.45300		293.20	Isothermal (vapor + liquid) equilibria of maleic anhydride + di-isobutyl hexahydrophthalate and maleic anhydride + di-n-butyl phthalate systems at T= (413.2, 433.2 and 453.2) K
rfi	1.45300		293.10	Isobaric vapor liquid equilibria of the binary system maleic anhydride and di-isobutyl hexahydrophthalate at 2.67, 5.33 and 8.00 kPa

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Isobaric vapor liquid equilibria of the binary system maleic anhydride and di-isobutyl hexahydrophthalate at 2.67, 5.33 and 8.00 kPa:	https://www.doi.org/10.1016/j.fluid.2005.03.019
Isothermal (vapor + liquid) equilibria of maleic anhydride + di-isobutyl hexahydrophthalate and maleic anhydride + di-n-butyl phthalate systems at T= (413.2, 433.2 and 453.2) K:	https://www.doi.org/10.1016/j.jct.2005.10.012
Liquid-Liquid Equilibria for the Binary Systems (Water + Di-n-butyl Phthalate), (Water + Di-n-butyl Phthalate) and (Water + Di-isobutyl Hexahydrophthalate) from (298.2 to 348.2) K:	https://www.doi.org/10.1021/je050382u
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339424&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume