1,2-Cyclohexanedicarboxylic acid, cyclobutyl isobutyl ester

Inchi: InChI=1S/C16H26O4/c1-11(2)10-19-15(17)13-8-3-4-9-14(13)16(18)20-12-6-5-7-12/h11-1

InchiKey: IMKSHWZMRNELNK-UHFFFAOYSA-N

Formula: C16H26O4

SMILES: CC(C)COC(=O)C1CCCCC1C(=O)OC1CCC1

Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-321.05	kJ/mol	Joback Method
hf	-767.83	kJ/mol	Joback Method
hfus	28.19	kJ/mol	Joback Method
hvap	69.34	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.088		Crippen Method
mcvol	229.460	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
rinpol	1917.00		NIST Webbook
rinpol	1917.00		NIST Webbook
tb	743.51	K	Joback Method
tc	958.53	K	Joback Method
tf	416.96	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.49	J/mol×K	743.51	Joback Method
cpg	740.51	J/mol×K	779.35	Joback Method
cpg	759.11	J/mol×K	815.18	Joback Method
cpg	776.33	J/mol×K	851.02	Joback Method
cpg	792.18	J/mol×K	886.86	Joback Method
cpg	806.70	J/mol×K	922.69	Joback Method
cpg	819.91	J/mol×K	958.53	Joback Method
dvisc	0.0021980	Pa×s	416.96	Joback Method

dvisc	0.0012067	Pa×s	471.39	Joback Method
dvisc	0.0007501	Pa×s	525.81	Joback Method
dvisc	0.0005097	Pa×s	580.24	Joback Method
dvisc	0.0003701	Pa×s	634.66	Joback Method
dvisc	0.0002827	Pa×s	689.09	Joback Method
dvisc	0.0002246	Pa×s	743.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339750&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume