1,2-Cyclohexanedicarboxylic acid, 2-cyclohexylethyl isobutyl ester

Inchi: InChI=1S/C20H34O4/c1-15(2)14-24-20(22)18-11-7-6-10-17(18)19(21)23-13-12-16-8-4-3

InchiKey: ZRSBXFIJIXOIEI-UHFFFAOYSA-N

Formula: C20H34O4

SMILES: CC(C)COC(=O)C1CCCCC1C(=O)OCCC1CCCCC1

Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-311.57	kJ/mol	Joback Method
hf	-862.71	kJ/mol	Joback Method
hfus	34.35	kJ/mol	Joback Method
hvap	78.59	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.506		Crippen Method
mcvol	285.820	ml/mol	McGowan Method
pc	1412.25	kPa	Joback Method
rinpol	2357.00		NIST Webbook
rinpol	2357.00		NIST Webbook
tb	843.57	K	Joback Method
tc	1060.05	K	Joback Method
tf	455.00	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.21	J/mol×K	843.57	Joback Method
cpg	987.73	J/mol×K	879.65	Joback Method
cpg	1006.48	J/mol×K	915.73	Joback Method
cpg	1023.49	J/mol×K	951.81	Joback Method
cpg	1038.78	J/mol×K	987.89	Joback Method
cpg	1052.39	J/mol×K	1023.97	Joback Method
cpg	1064.33	J/mol×K	1060.05	Joback Method
dvisc	0.0013583	Pa×s	455.00	Joback Method

dvisc	0.0006024	Pa×s	519.76	Joback Method
dvisc	0.0003199	Pa×s	584.52	Joback Method
dvisc	0.0001928	Pa×s	649.28	Joback Method
dvisc	0.0001273	Pa×s	714.05	Joback Method
dvisc	0.0000901	Pa×s	778.81	Joback Method
dvisc	0.0000672	Pa×s	843.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339724&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