Dicyclohexyl glutarate

Other names: Dicyclohexyl pentanedioate
Inchi: InChI=1S/C17H28O4/c18-16(20-14-8-3-1-4-9-14)12-7-13-17(19)21-15-10-5-2-6-11-15/h1
InchiKey: QMHOJBZGLTYRED-UHFFFAOYSA-N
Formula: C17H28O4
SMILES: O=C(CCCC(=O)OC1CCCCC1)OC1CCCCC1
Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-326.68	kJ/mol	Joback Method
hf	-775.17	kJ/mol	Joback Method
hfus	29.03	kJ/mol	Joback Method
hvap	72.61	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.909		Crippen Method
mcvol	243.550	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	2133.00		NIST Webbook
rinpol	2133.00		NIST Webbook
rinpol	2148.00		NIST Webbook
rinpol	2158.00		NIST Webbook
rinpol	2124.00		NIST Webbook
rinpol	2124.00		NIST Webbook
rinpol	2140.00		NIST Webbook
tb	780.04	K	Joback Method
tc	1000.03	K	Joback Method
tf	440.43	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	783.13	J/mol×K	780.04	Joback Method
cpg	803.50	J/mol×K	816.70	Joback Method

cpg	822.25	J/mol×K	853.37	Joback Method
cpg	839.40	J/mol×K	890.03	Joback Method
cpg	855.00	J/mol×K	926.70	Joback Method
cpg	869.04	J/mol×K	963.36	Joback Method
cpg	881.57	J/mol×K	1000.03	Joback Method
dvisc	0.0015318	Pa×s	440.43	Joback Method
dvisc	0.0007244	Pa×s	497.03	Joback Method
dvisc	0.0003993	Pa×s	553.63	Joback Method
dvisc	0.0002458	Pa×s	610.24	Joback Method
dvisc	0.0001643	Pa×s	666.84	Joback Method
dvisc	0.0001169	Pa×s	723.44	Joback Method
dvisc	0.0000875	Pa×s	780.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R542486&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume