Glutaric acid, cyclohexylmethyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C19H34O4/c1-4-9-17(15(2)3)23-19(21)13-8-12-18(20)22-14-16-10-6-5-7-11-16

InchiKey: ASKZOIGTILEXPG-UHFFFAOYSA-N

Formula: C19H34O4

SMILES: CCCC(OC(=O)CCCC(=O)OCC1CCCCC1)C(C)C

Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-339.17	kJ/mol	Joback Method
hf	-881.33	kJ/mol	Joback Method
hfus	35.33	kJ/mol	Joback Method
hvap	75.85	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.648		Crippen Method
mcvol	282.590	ml/mol	McGowan Method
pc	1342.74	kPa	Joback Method
rinpol	2179.00		NIST Webbook
rinpol	2179.00		NIST Webbook
tb	805.37	K	Joback Method
tc	1004.36	K	Joback Method
tf	425.59	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.75	J/mol×K	805.37	Joback Method
cpg	925.89	J/mol×K	838.54	Joback Method
cpg	943.73	J/mol×K	871.70	Joback Method
cpg	960.27	J/mol×K	904.87	Joback Method
cpg	975.54	J/mol×K	938.03	Joback Method
cpg	989.57	J/mol×K	971.20	Joback Method
cpg	1002.36	J/mol×K	1004.36	Joback Method
dvisc	0.0015521	Pa×s	425.59	Joback Method

dvisc	0.0006163	Pa×s	488.89	Joback Method
dvisc	0.0003025	Pa×s	552.18	Joback Method
dvisc	0.0001718	Pa×s	615.48	Joback Method
dvisc	0.0001085	Pa×s	678.78	Joback Method
dvisc	0.0000741	Pa×s	742.07	Joback Method
dvisc	0.0000537	Pa×s	805.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393734&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

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