Glutaric acid, cyclohexylmethyl 2,4-dimethylpent-3-yl ester

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

InchiKey: YZKQHJSZAPRAPY-UHFFFAOYSA-N

Formula: C19H34O4

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

Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-341.61	kJ/mol	Joback Method
hf	-886.61	kJ/mol	Joback Method
hfus	31.81	kJ/mol	Joback Method
hvap	75.47	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.504		Crippen Method
mcvol	282.590	ml/mol	McGowan Method
pc	1350.65	kPa	Joback Method
rinpol	2177.00		NIST Webbook
rinpol	2177.00		NIST Webbook
tb	804.93	K	Joback Method
tc	1006.12	K	Joback Method
tf	410.59	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.23	J/mol×K	804.93	Joback Method
cpg	926.59	J/mol×K	838.46	Joback Method
cpg	944.60	J/mol×K	871.99	Joback Method
cpg	961.27	J/mol×K	905.52	Joback Method
cpg	976.64	J/mol×K	939.05	Joback Method
cpg	990.72	J/mol×K	972.59	Joback Method
cpg	1003.53	J/mol×K	1006.12	Joback Method
dvisc	0.0019316	Pa×s	410.59	Joback Method

dvisc	0.0006875	Pa×s	476.31	Joback Method
dvisc	0.0003144	Pa×s	542.04	Joback Method
dvisc	0.0001703	Pa×s	607.76	Joback Method
dvisc	0.0001039	Pa×s	673.48	Joback Method
dvisc	0.0000693	Pa×s	739.21	Joback Method
dvisc	0.0000493	Pa×s	804.93	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=U393479&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