Glutaric acid, 3,5-dimethylcyclohexyl hept-2-yl ester

Inchi: InChI=1S/C20H36O4/c1-5-6-7-9-17(4)23-19(21)10-8-11-20(22)24-18-13-15(2)12-16(3)14

InchiKey: FNCTWSPYQAQULF-UHFFFAOYSA-N

Formula: C20H36O4

SMILES: CCCCCC(C)OC(=O)CCCC(=O)OC1CC(C)CC(C)C1

Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	-343.73	kJ/mol	Joback Method
hf	-937.37	kJ/mol	Joback Method
hfus	43.58	kJ/mol	Joback Method
hvap	77.85	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	5.037		Crippen Method
mcvol	296.680	ml/mol	McGowan Method
pc	1189.88	kPa	Joback Method
rinpol	2205.00		NIST Webbook
rinpol	2205.00		NIST Webbook
tb	819.35	K	Joback Method
tc	1015.85	K	Joback Method
tf	443.38	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	973.03	J/mol×K	819.35	Joback Method
cpg	992.83	J/mol×K	852.10	Joback Method
cpg	1011.23	J/mol×K	884.85	Joback Method
cpg	1028.27	J/mol×K	917.60	Joback Method
cpg	1043.94	J/mol×K	950.35	Joback Method
cpg	1058.25	J/mol×K	983.10	Joback Method
cpg	1071.23	J/mol×K	1015.85	Joback Method
dvisc	0.0012193	Pa×s	443.38	Joback Method

dvisc	0.0005904	Pa×s	506.04	Joback Method
dvisc	0.0003354	Pa×s	568.70	Joback Method
dvisc	0.0002132	Pa×s	631.37	Joback Method
dvisc	0.0001470	Pa×s	694.03	Joback Method
dvisc	0.0001079	Pa×s	756.69	Joback Method
dvisc	0.0000830	Pa×s	819.35	Joback Method

Sources

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=U405409&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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