Glutaric acid, heptyl 4-methoxy-2-methylbutyl ester

Inchi: InChI=1S/C18H34O5/c1-4-5-6-7-8-13-22-17(19)10-9-11-18(20)23-15-16(2)12-14-21-3/h1

InchiKey: HTUIEUJRFGBDOM-UHFFFAOYSA-N

Formula: C18H34O5

SMILES: CCCCCCCOC(=O)CCCC(=O)OCC(C)CCOC

Mol. weight [g/mol]: 330.46

Physical Properties

Property code	Value	Unit	Source
gf	-474.60	kJ/mol	Joback Method
hf	-1041.95	kJ/mol	Joback Method
hfus	45.61	kJ/mol	Joback Method
hvap	76.00	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.886		Crippen Method
mcvol	285.230	ml/mol	McGowan Method
pc	1219.99	kPa	Joback Method
rinpol	2277.00		NIST Webbook
tb	785.80	K	Joback Method
tc	967.95	K	Joback Method
tf	444.17	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.97	J/mol×K	785.80	Joback Method
cpg	898.29	J/mol×K	816.16	Joback Method
cpg	914.61	J/mol×K	846.52	Joback Method
cpg	929.94	J/mol×K	876.87	Joback Method
cpg	944.29	J/mol×K	907.23	Joback Method
cpg	957.65	J/mol×K	937.59	Joback Method
cpg	970.03	J/mol×K	967.95	Joback Method
dvisc	0.0008380	Pa×s	444.17	Joback Method
dvisc	0.0003989	Pa×s	501.11	Joback Method

dvisc	0.0002209	Pa×s	558.05	Joback Method
dvisc	0.0001365	Pa×s	614.98	Joback Method
dvisc	0.0000915	Pa×s	671.92	Joback Method
dvisc	0.0000653	Pa×s	728.86	Joback Method
dvisc	0.0000489	Pa×s	785.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359416&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