Glutaric acid, heptyl hexyl ester

Inchi: InChI=1S/C18H34O4/c1-3-5-7-9-11-16-22-18(20)14-12-13-17(19)21-15-10-8-6-4-2/h3-16
InchiKey: JGIRBBZTOHGRCQ-UHFFFAOYSA-N
Formula: C18H34O4
SMILES: CCCCCCCOC(=O)CCCC(=O)OCCCCCC
Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
gf	-367.16	kJ/mol	Joback Method
hf	-904.45	kJ/mol	Joback Method
hfus	47.95	kJ/mol	Joback Method
hvap	73.97	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.794		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1227.70	kPa	Joback Method
rinpol	2184.00		NIST Webbook
tb	763.82	K	Joback Method
tc	942.53	K	Joback Method
tf	436.94	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.49	J/mol×K	763.82	Joback Method
cpg	866.90	J/mol×K	793.61	Joback Method
cpg	883.40	J/mol×K	823.39	Joback Method
cpg	898.98	J/mol×K	853.18	Joback Method
cpg	913.68	J/mol×K	882.96	Joback Method
cpg	927.49	J/mol×K	912.75	Joback Method
cpg	940.44	J/mol×K	942.53	Joback Method
dvisc	0.0010365	Pa×s	436.94	Joback Method
dvisc	0.0005169	Pa×s	491.42	Joback Method

dvisc	0.0002962	Pa×s	545.90	Joback Method
dvisc	0.0001878	Pa×s	600.38	Joback Method
dvisc	0.0001284	Pa×s	654.86	Joback Method
dvisc	0.0000931	Pa×s	709.34	Joback Method
dvisc	0.0000707	Pa×s	763.82	Joback Method

Sources

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=U358327&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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