Glutaric acid, heptyl 3-methylbut-2-enyl ester

Inchi: InChI=1S/C17H30O4/c1-4-5-6-7-8-13-20-16(18)10-9-11-17(19)21-14-12-15(2)3/h12H,4-1
InchiKey: ACDDLJGMLUDCCD-UHFFFAOYSA-N
Formula: C17H30O4
SMILES: CCCCCCCOC(=O)CCCC(=O)OCC=C(C)C
Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-303.91	kJ/mol	Joback Method
hf	-776.38	kJ/mol	Joback Method
hfus	44.25	kJ/mol	Joback Method
hvap	71.79	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.180		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1370.73	kPa	Joback Method
rinpol	2106.00		NIST Webbook
rinpol	2106.00		NIST Webbook
tb	744.98	K	Joback Method
tc	927.61	K	Joback Method
tf	406.63	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.93	J/mol×K	744.98	Joback Method
cpg	783.53	J/mol×K	775.42	Joback Method
cpg	799.26	J/mol×K	805.86	Joback Method
cpg	814.15	J/mol×K	836.30	Joback Method
cpg	828.22	J/mol×K	866.73	Joback Method
cpg	841.48	J/mol×K	897.17	Joback Method
cpg	853.95	J/mol×K	927.61	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=U360091&Units=SI

Legend

cpg:	Ideal gas heat capacity
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