Glutaric acid, 3-methylbut-2-en-1-yl 3-octyl ester

Inchi: InChI=1S/C18H32O4/c1-5-7-8-10-16(6-2)22-18(20)12-9-11-17(19)21-14-13-15(3)4/h13,1
InchiKey: OGRURBAORLKAHA-UHFFFAOYSA-N
Formula: C18H32O4
SMILES: CCCCCC(CC)OC(=O)CCCC(=O)OCC=C(C)C
Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-297.93	kJ/mol	Joback Method
hf	-802.30	kJ/mol	Joback Method
hfus	43.32	kJ/mol	Joback Method
hvap	73.62	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.568		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1285.59	kPa	Joback Method
rinpol	2004.00		NIST Webbook
rinpol	2004.00		NIST Webbook
tb	767.42	K	Joback Method
tc	952.49	K	Joback Method
tf	402.90	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.34	J/mol×K	767.42	Joback Method
cpg	842.48	J/mol×K	798.27	Joback Method
cpg	858.70	J/mol×K	829.11	Joback Method
cpg	874.00	J/mol×K	859.96	Joback Method
cpg	888.43	J/mol×K	890.80	Joback Method
cpg	901.98	J/mol×K	921.65	Joback Method
cpg	914.70	J/mol×K	952.49	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=U391558&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