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

Inchi: InChI=1S/C18H32O4/c1-4-5-6-7-8-9-14-21-17(19)11-10-12-18(20)22-15-13-16(2)3/h13H
InchiKey: JEIDNXVGFCEODH-UHFFFAOYSA-N
Formula: C18H32O4
SMILES: CCCCCCCCOC(=O)CCCC(=O)OCC=C(C)C
Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-295.49	kJ/mol	Joback Method
hf	-797.02	kJ/mol	Joback Method
hfus	46.84	kJ/mol	Joback Method
hvap	74.01	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.570		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1278.25	kPa	Joback Method
rinpol	2202.00		NIST Webbook
rinpol	2202.00		NIST Webbook
tb	767.86	K	Joback Method
tc	951.28	K	Joback Method
tf	417.90	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.84	J/mol×K	767.86	Joback Method
cpg	841.82	J/mol×K	798.43	Joback Method
cpg	857.90	J/mol×K	829.00	Joback Method
cpg	873.09	J/mol×K	859.57	Joback Method
cpg	887.43	J/mol×K	890.14	Joback Method
cpg	900.92	J/mol×K	920.71	Joback Method
cpg	913.59	J/mol×K	951.28	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=U360092&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