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

Inchi: InChI=1S/C22H40O4/c1-4-5-6-7-8-9-10-11-12-13-18-25-21(23)15-14-16-22(24)26-19-17
InchiKey: JFIIRXXNZDZCDQ-UHFFFAOYSA-N
Formula: C22H40O4
SMILES: CCCCCCCCCCCCOC(=O)CCCC(=O)OCC=C(C)C
Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-261.81	kJ/mol	Joback Method
hf	-879.58	kJ/mol	Joback Method
hfus	57.20	kJ/mol	Joback Method
hvap	82.92	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.130		Crippen Method
mcvol	331.420	ml/mol	McGowan Method
pc	988.26	kPa	Joback Method
rinpol	2615.00		NIST Webbook
tb	859.38	K	Joback Method
tc	1052.77	K	Joback Method
tf	462.98	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1065.44	J/mol×K	859.38	Joback Method
cpg	1084.03	J/mol×K	891.61	Joback Method
cpg	1101.49	J/mol×K	923.84	Joback Method
cpg	1117.88	J/mol×K	956.08	Joback Method
cpg	1133.21	J/mol×K	988.31	Joback Method
cpg	1147.52	J/mol×K	1020.54	Joback Method
cpg	1160.85	J/mol×K	1052.77	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=U360096&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