Glutaric acid, dodec-9-ynyl pentyl ester

Inchi: InChI=1S/C22H38O4/c1-3-5-7-8-9-10-11-12-13-15-20-26-22(24)18-16-17-21(23)25-19-1
InchiKey: NXJAJUIJBJIXNH-UHFFFAOYSA-N
Formula: C22H38O4
SMILES: CCC#CCCCCCCCCOC(=O)CCCC(=O)OCCCCC
Mol. weight [g/mol]: 366.53

Physical Properties

Property code	Value	Unit	Source
gf	-130.68	kJ/mol	Joback Method
hf	-714.71	kJ/mol	Joback Method
hfus	61.43	kJ/mol	Joback Method
hvap	85.03	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	5.577		Crippen Method
mcvol	327.120	ml/mol	McGowan Method
pc	1055.51	kPa	Joback Method
rinpol	2659.00		NIST Webbook
rinpol	2659.00		NIST Webbook
tb	864.34	K	Joback Method
tc	1060.10	K	Joback Method
tf	588.12	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1040.92	J/mol×K	864.34	Joback Method
cpg	1058.93	J/mol×K	896.97	Joback Method
cpg	1075.77	J/mol×K	929.59	Joback Method
cpg	1091.47	J/mol×K	962.22	Joback Method
cpg	1106.04	J/mol×K	994.85	Joback Method
cpg	1119.52	J/mol×K	1027.47	Joback Method
cpg	1131.91	J/mol×K	1060.10	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=U359787&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