Glutaric acid, 8-chlorooctyl dodec-9-yn-1-yl ester

Inchi: InChI=1S/C25H43ClO4/c1-2-3-4-5-6-7-8-10-13-16-22-29-24(27)19-18-20-25(28)30-23-17
InchiKey: FYUFNVNTOGXIBP-UHFFFAOYSA-N
Formula: C25H43ClO4
SMILES: CCC#CCCCCCCCCOC(=O)CCCC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 443.06

Physical Properties

Property code	Value	Unit	Source
gf	-117.35	kJ/mol	Joback Method
hf	-792.37	kJ/mol	Joback Method
hfus	73.40	kJ/mol	Joback Method
hvap	96.09	kJ/mol	Joback Method
log10ws	-7.96		Crippen Method
logp	6.967		Crippen Method
mcvol	381.630	ml/mol	McGowan Method
pc	863.53	kPa	Joback Method
rinpol	3227.00		NIST Webbook
tb	970.41	K	Joback Method
tc	1189.71	K	Joback Method
tf	651.85	K	Joback Method
vc	1.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1256.50	J/mol×K	970.41	Joback Method
cpg	1274.62	J/mol×K	1006.96	Joback Method
cpg	1291.25	J/mol×K	1043.51	Joback Method
cpg	1306.42	J/mol×K	1080.06	Joback Method
cpg	1320.17	J/mol×K	1116.61	Joback Method
cpg	1332.55	J/mol×K	1153.16	Joback Method
cpg	1343.60	J/mol×K	1189.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393946&Units=SI
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

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