Glutaric acid, 8-chlorooctyl non-5-yn-3-yl ester

Inchi: InChI=1S/C22H37ClO4/c1-3-5-6-11-15-20(4-2)27-22(25)17-14-16-21(24)26-19-13-10-8-7
InchiKey: MJQBFGSJEBIVMS-UHFFFAOYSA-N
Formula: C22H37ClO4
SMILES: CCCC#CCC(CC)OC(=O)CCCC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 400.98

Physical Properties

Property code	Value	Unit	Source
gf	-145.05	kJ/mol	Joback Method
hf	-735.73	kJ/mol	Joback Method
hfus	62.11	kJ/mol	Joback Method
hvap	89.03	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.795		Crippen Method
mcvol	339.360	ml/mol	McGowan Method
pc	1035.90	kPa	Joback Method
rinpol	2779.00		NIST Webbook
rinpol	2779.00		NIST Webbook
tb	901.33	K	Joback Method
tc	1104.72	K	Joback Method
tf	603.04	K	Joback Method
vc	1.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1070.96	J/mol×K	901.33	Joback Method
cpg	1087.96	J/mol×K	935.23	Joback Method
cpg	1103.74	J/mol×K	969.13	Joback Method
cpg	1118.31	J/mol×K	1003.03	Joback Method
cpg	1131.70	J/mol×K	1036.92	Joback Method
cpg	1143.94	J/mol×K	1070.82	Joback Method
cpg	1155.05	J/mol×K	1104.72	Joback Method

Sources

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=U393958&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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