Glutaric acid, 8-chlorooctyl 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C24H39ClO4/c1-5-13-21(4)22(17-16-20(2)3)29-24(27)15-12-14-23(26)28-19-1

InchiKey: RYVQVUMQJFFIQP-UHFFFAOYSA-N

Formula: C24H39ClO4

SMILES: C=C(C)C#CC(OC(=O)CCCC(=O)OCCCCCCCCCCl)C(C)CCC

Mol. weight [g/mol]: 427.02

Physical Properties

Property code	Value	Unit	Source
gf	-51.36	kJ/mol	Joback Method
hf	-666.65	kJ/mol	Joback Method
hfus	61.17	kJ/mol	Joback Method
hvap	92.50	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	6.207		Crippen Method
mcvol	363.240	ml/mol	McGowan Method
pc	950.25	kPa	Joback Method
rinpol	2807.00		NIST Webbook
rinpol	2807.00		NIST Webbook
tb	943.21	K	Joback Method
tc	1155.06	K	Joback Method
tf	594.86	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1165.04	J/mol×K	943.21	Joback Method
cpg	1182.20	J/mol×K	978.52	Joback Method
cpg	1198.04	J/mol×K	1013.83	Joback Method
cpg	1212.58	J/mol×K	1049.13	Joback Method
cpg	1225.87	J/mol×K	1084.44	Joback Method
cpg	1237.96	J/mol×K	1119.75	Joback Method
cpg	1248.87	J/mol×K	1155.06	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=U393968&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