Glutaric acid, tridec-2-yn-1-yl 8-chlorooctyl ester

Inchi: InChI=1S/C26H45ClO4/c1-2-3-4-5-6-7-8-9-11-14-17-23-30-25(28)20-19-21-26(29)31-24-

InchiKey: ZEYFKDFMUIOFRN-UHFFFAOYSA-N

Formula: C26H45ClO4

SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)OCCCCCCCCCl

Mol. weight [g/mol]: 457.09

Physical Properties

Property code	Value	Unit	Source
gf	-108.93	kJ/mol	Joback Method
hf	-813.01	kJ/mol	Joback Method
hfus	75.99	kJ/mol	Joback Method
hvap	98.32	kJ/mol	Joback Method
log10ws	-8.38		Crippen Method
logp	7.357		Crippen Method
mcvol	395.720	ml/mol	McGowan Method
pc	816.79	kPa	Joback Method
rinpol	3304.00		NIST Webbook
tb	993.29	K	Joback Method
tc	1220.20	K	Joback Method
tf	663.12	K	Joback Method
vc	1.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1319.47	J/mol×K	993.29	Joback Method
cpg	1338.03	J/mol×K	1031.11	Joback Method
cpg	1354.97	J/mol×K	1068.93	Joback Method
cpg	1370.33	J/mol×K	1106.74	Joback Method
cpg	1384.16	J/mol×K	1144.56	Joback Method
cpg	1396.52	J/mol×K	1182.38	Joback Method
cpg	1407.46	J/mol×K	1220.20	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=U393468&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