Glutaric acid, but-3-yn-2-yl 8-chlorooctyl ester

Inchi: InChI=1S/C17H27ClO4/c1-3-15(2)22-17(20)12-10-11-16(19)21-14-9-7-5-4-6-8-13-18/h1,
InchiKey: JWRZEMBOPTYJLN-UHFFFAOYSA-N
Formula: C17H27ClO4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 330.85

Physical Properties

Property code	Value	Unit	Source
gf	-166.88	kJ/mol	Joback Method
hf	-612.93	kJ/mol	Joback Method
hfus	49.01	kJ/mol	Joback Method
hvap	75.60	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	3.844		Crippen Method
mcvol	268.910	ml/mol	McGowan Method
pc	1435.89	kPa	Joback Method
rinpol	2268.00		NIST Webbook
rinpol	2268.00		NIST Webbook
tb	768.05	K	Joback Method
tc	956.98	K	Joback Method
tf	487.56	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.93	J/mol×K	768.05	Joback Method
cpg	785.22	J/mol×K	799.54	Joback Method
cpg	799.62	J/mol×K	831.03	Joback Method
cpg	813.15	J/mol×K	862.52	Joback Method
cpg	825.84	J/mol×K	894.01	Joback Method
cpg	837.70	J/mol×K	925.49	Joback Method
cpg	848.74	J/mol×K	956.98	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=U393458&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