Glutaric acid, hex-4-yn-3-yl 8-chlorooctyl ester

Inchi: InChI=1S/C19H31ClO4/c1-3-12-17(4-2)24-19(22)14-11-13-18(21)23-16-10-8-6-5-7-9-15-
InchiKey: CSLXNBVBLUZIRA-UHFFFAOYSA-N
Formula: C19H31ClO4
SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 358.90

Physical Properties

Property code	Value	Unit	Source
gf	-170.31	kJ/mol	Joback Method
hf	-673.81	kJ/mol	Joback Method
hfus	54.34	kJ/mol	Joback Method
hvap	82.35	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	4.624		Crippen Method
mcvol	297.090	ml/mol	McGowan Method
pc	1258.37	kPa	Joback Method
rinpol	2515.00		NIST Webbook
rinpol	2515.00		NIST Webbook
tb	832.69	K	Joback Method
tc	1028.98	K	Joback Method
tf	569.23	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	890.61	J/mol×K	832.69	Joback Method
cpg	906.74	J/mol×K	865.41	Joback Method
cpg	921.82	J/mol×K	898.12	Joback Method
cpg	935.88	J/mol×K	930.84	Joback Method
cpg	948.92	J/mol×K	963.55	Joback Method
cpg	960.97	J/mol×K	996.27	Joback Method
cpg	972.03	J/mol×K	1028.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393463&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