Glutaric acid, hex-4-yn-3-yl 2,6-dichlorophenyl ester

Inchi: InChI=1S/C17H18Cl2O4/c1-3-7-12(4-2)22-15(20)10-6-11-16(21)23-17-13(18)8-5-9-14(1
InchiKey: CZQARZBAUNBDFU-UHFFFAOYSA-N
Formula: C17H18Cl2O4
SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 357.23

Physical Properties

Property code	Value	Unit	Source
gf	-105.93	kJ/mol	Joback Method
hf	-434.68	kJ/mol	Joback Method
hfus	46.62	kJ/mol	Joback Method
hvap	85.88	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	4.414		Crippen Method
mcvol	257.390	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	2428.00		NIST Webbook
rinpol	2428.00		NIST Webbook
tb	861.00	K	Joback Method
tc	1088.30	K	Joback Method
tf	628.07	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.74	J/mol×K	861.00	Joback Method
cpg	715.15	J/mol×K	898.88	Joback Method
cpg	726.43	J/mol×K	936.77	Joback Method
cpg	736.59	J/mol×K	974.65	Joback Method
cpg	745.64	J/mol×K	1012.53	Joback Method
cpg	753.58	J/mol×K	1050.42	Joback Method
cpg	760.45	J/mol×K	1088.30	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=U390256&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