

Glutaric acid, hex-4-yn-3-yl 2,5-dichlorophenyl ester

Inchi:	InChI=1S/C17H18Cl2O4/c1-3-6-13(4-2)22-16(20)7-5-8-17(21)23-15-11-12(18)9-10-14(19)
InchiKey:	FYTHNALNGUEGKO-UHFFFAOYSA-N
Formula:	C17H18Cl2O4
SMILES:	CC#CC(CC)OC(=O)CCCC(=O)Oc1cc(Cl)ccc1Cl
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
mvol	257.390	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	2435.00		NIST Webbook
rinpol	2435.00		NIST Webbook
tb	861.00	K	Joback Method
tc	1088.30	K	Joback Method
tf	628.07	K	Joback Method
vc	0.982	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U392056&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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