Glutaric acid, 3-methylbut-2-en-1-yl 2,6-dichlorophenyl ester

Inchi: InChI=1S/C16H18Cl2O4/c1-11(2)9-10-21-14(19)7-4-8-15(20)22-16-12(17)5-3-6-13(16)18

InchiKey: PYQWPRGJYOYZPM-UHFFFAOYSA-N

Formula: C16H18Cl2O4

SMILES: CC(C)=CCOC(=O)CCCC(=O)Oc1c(Cl)cccc1Cl

Mol. weight [g/mol]: 345.22

Physical Properties

Property code	Value	Unit	Source
gf	-243.04	kJ/mol	Joback Method
hf	-573.63	kJ/mol	Joback Method
hfus	43.32	kJ/mol	Joback Method
hvap	81.93	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.578		Crippen Method
mcvol	247.600	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	2378.00		NIST Webbook
rinpol	2378.00		NIST Webbook
tb	833.60	K	Joback Method
tc	1051.90	K	Joback Method
tf	506.66	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.81	J/mol×K	833.60	Joback Method
cpg	684.23	J/mol×K	869.98	Joback Method
cpg	695.68	J/mol×K	906.37	Joback Method
cpg	706.19	J/mol×K	942.75	Joback Method
cpg	715.80	J/mol×K	979.13	Joback Method
cpg	724.52	J/mol×K	1015.52	Joback Method
cpg	732.38	J/mol×K	1051.90	Joback Method

Sources

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=U390254&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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