Glutaric acid, 1-cyclopentylethyl 2,3-dichlorophenyl ester

Inchi: InChI=1S/C18H22Cl2O4/c1-12(13-6-2-3-7-13)23-16(21)10-5-11-17(22)24-15-9-4-8-14(19

InchiKey: MWJCIDWUJHZMGV-UHFFFAOYSA-N

Formula: C18H22Cl2O4

SMILES: CC(OC(=O)CCCC(=O)Oc1cccc(Cl)c1Cl)C1CCCC1

Mol. weight [g/mol]: 373.27

Physical Properties

Property code	Value	Unit	Source
gf	-263.76	kJ/mol	Joback Method
hf	-667.14	kJ/mol	Joback Method
hfus	40.02	kJ/mol	Joback Method
hvap	86.21	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.191		Crippen Method
mcvol	269.220	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	2650.00		NIST Webbook
rinpol	2650.00		NIST Webbook
tb	890.16	K	Joback Method
tc	1118.60	K	Joback Method
tf	544.14	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.59	J/mol×K	890.16	Joback Method
cpg	816.39	J/mol×K	928.23	Joback Method
cpg	828.84	J/mol×K	966.31	Joback Method
cpg	839.99	J/mol×K	1004.38	Joback Method
cpg	849.86	J/mol×K	1042.45	Joback Method
cpg	858.50	J/mol×K	1080.53	Joback Method
cpg	865.93	J/mol×K	1118.60	Joback Method
dvisc	0.0006284	Pa×s	544.14	Joback Method

dvisc	0.0003729	Pa×s	601.81	Joback Method
dvisc	0.0002424	Pa×s	659.48	Joback Method
dvisc	0.0001689	Pa×s	717.15	Joback Method
dvisc	0.0001241	Pa×s	774.82	Joback Method
dvisc	0.0000952	Pa×s	832.49	Joback Method
dvisc	0.0000756	Pa×s	890.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405468&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
dvisc:	Dynamic viscosity
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