Glutaric acid, 2,2-dichloroethyl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C16H20Cl2O5/c1-11(2)22-12-6-3-4-7-13(12)23-16(20)9-5-8-15(19)21-10-14(17

InchiKey: KRHBCQDDKAIZMB-UHFFFAOYSA-N

Formula: C16H20Cl2O5

SMILES: CC(C)Oc1ccccc1OC(=O)CCCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 363.23

Physical Properties

Property code	Value	Unit	Source
gf	-414.96	kJ/mol	Joback Method
hf	-812.37	kJ/mol	Joback Method
hfus	38.96	kJ/mol	Joback Method
hvap	82.86	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	3.896		Crippen Method
mcvol	257.770	ml/mol	McGowan Method
pc	1706.12	kPa	Joback Method
rinpol	2384.00		NIST Webbook
rinpol	2384.00		NIST Webbook
tb	846.12	K	Joback Method
tc	1060.29	K	Joback Method
tf	505.41	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	727.93	J/mol×K	846.12	Joback Method
cpg	779.84	J/mol×K	1024.59	Joback Method
cpg	771.73	J/mol×K	988.90	Joback Method
cpg	762.49	J/mol×K	953.20	Joback Method
cpg	752.11	J/mol×K	917.51	Joback Method
cpg	740.59	J/mol×K	881.81	Joback Method
cpg	786.81	J/mol×K	1060.29	Joback Method
dvisc	0.0000453	Pa×s	846.12	Joback Method

dvisc	0.0000589	Pa×s	789.34	Joback Method
dvisc	0.0000797	Pa×s	732.55	Joback Method
dvisc	0.0001134	Pa×s	675.76	Joback Method
dvisc	0.0001721	Pa×s	618.98	Joback Method
dvisc	0.0002843	Pa×s	562.20	Joback Method
dvisc	0.0005258	Pa×s	505.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391870&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