Glutaric acid, 2,2-dichloroethyl 2-isopropylphenyl ester

Inchi: InChI=1S/C16H20Cl2O4/c1-11(2)12-6-3-4-7-13(12)22-16(20)9-5-8-15(19)21-10-14(17)18

InchiKey: UAOBRRMQORHYBP-UHFFFAOYSA-N

Formula: C16H20Cl2O4

SMILES: CC(C)c1ccccc1OC(=O)CCCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 347.23

Physical Properties

Property code	Value	Unit	Source
gf	-309.96	kJ/mol	Joback Method
hf	-680.15	kJ/mol	Joback Method
hfus	37.77	kJ/mol	Joback Method
hvap	80.45	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.233		Crippen Method
mcvol	251.900	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	2296.00		NIST Webbook
rinpol	2296.00		NIST Webbook
tb	823.70	K	Joback Method
tc	1038.56	K	Joback Method
tf	483.18	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.26	J/mol×K	823.70	Joback Method
cpg	714.43	J/mol×K	859.51	Joback Method
cpg	726.52	J/mol×K	895.32	Joback Method
cpg	737.56	J/mol×K	931.13	Joback Method
cpg	747.55	J/mol×K	966.94	Joback Method
cpg	756.53	J/mol×K	1002.75	Joback Method
cpg	764.50	J/mol×K	1038.56	Joback Method
dvisc	0.0007599	Pa×s	483.18	Joback Method

dvisc	0.0003996	Pa×s	539.93	Joback Method
dvisc	0.0002375	Pa×s	596.69	Joback Method
dvisc	0.0001545	Pa×s	653.44	Joback Method
dvisc	0.0001077	Pa×s	710.19	Joback Method
dvisc	0.0000791	Pa×s	766.95	Joback Method
dvisc	0.0000607	Pa×s	823.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391916&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