Glutaric acid, 2,2-dichloroethyl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C15H18Cl2O6/c1-20-10-5-3-6-11(21-2)15(10)23-14(19)8-4-7-13(18)22-9-12(16

InchiKey: QFFCWRBUIPKUGD-UHFFFAOYSA-N

Formula: C15H18Cl2O6

SMILES: COc1cccc(OC)c1OC(=O)CCCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 365.21

Physical Properties

Property code	Value	Unit	Source
gf	-535.57	kJ/mol	Joback Method
hf	-930.14	kJ/mol	Joback Method
hfus	40.69	kJ/mol	Joback Method
hvap	84.10	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.126		Crippen Method
mcvol	249.550	ml/mol	McGowan Method
pc	1787.88	kPa	Joback Method
rinpol	2512.00		NIST Webbook
rinpol	2512.00		NIST Webbook
tb	851.08	K	Joback Method
tc	1064.18	K	Joback Method
tf	543.89	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.37	J/mol×K	851.08	Joback Method
cpg	743.25	J/mol×K	1028.67	Joback Method
cpg	736.26	J/mol×K	993.15	Joback Method
cpg	728.05	J/mol×K	957.63	Joback Method
cpg	718.66	J/mol×K	922.11	Joback Method
cpg	708.09	J/mol×K	886.60	Joback Method
cpg	749.01	J/mol×K	1064.18	Joback Method
dvisc	0.0000433	Pa×s	851.08	Joback Method

dvisc	0.0000543	Pa×s	799.88	Joback Method
dvisc	0.0000702	Pa×s	748.68	Joback Method
dvisc	0.0000944	Pa×s	697.48	Joback Method
dvisc	0.0001330	Pa×s	646.29	Joback Method
dvisc	0.0001986	Pa×s	595.09	Joback Method
dvisc	0.0003200	Pa×s	543.89	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392002&Units=SI

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

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