

Glutaric acid, 2,5-dichlorophenyl isohexyl ester

Inchi:	InChI=1S/C17H22Cl2O4/c1-12(2)5-4-10-22-16(20)6-3-7-17(21)23-15-11-13(18)8-9-14(19)
InchiKey:	KZDIASNAIWTFLLH-UHFFFAOYSA-N
Formula:	C17H22Cl2O4
SMILES:	CC(C)CCCOC(=O)CCCC(=O)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	361.26

Physical Properties

Property code	Value	Unit	Source
gf	-308.73	kJ/mol	Joback Method
hf	-706.98	kJ/mol	Joback Method
hfus	43.49	kJ/mol	Joback Method
hvap	83.73	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	5.048		Crippen Method
mcvol	265.990	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	2492.00		NIST Webbook
rinpol	2492.00		NIST Webbook
tb	852.00	K	Joback Method
tc	1063.90	K	Joback Method
tf	521.97	K	Joback Method
vc	1.020	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.82	J/molxK	852.00	Joback Method
cpg	768.99	J/molxK	887.32	Joback Method
cpg	781.08	J/molxK	922.63	Joback Method
cpg	792.11	J/molxK	957.95	Joback Method
cpg	802.10	J/molxK	993.26	Joback Method
cpg	811.05	J/molxK	1028.58	Joback Method
cpg	818.99	J/molxK	1063.90	Joback Method
dvisc	0.0005217	Paxs	521.97	Joback Method

dvisc	0.0003039	Paxs	576.98	Joback Method
dvisc	0.0001945	Paxs	631.98	Joback Method
dvisc	0.0001337	Paxs	686.99	Joback Method
dvisc	0.0000971	Paxs	741.99	Joback Method
dvisc	0.0000738	Paxs	797.00	Joback Method
dvisc	0.0000580	Paxs	852.00	Joback Method

Sources

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=U358997&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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