Glutaric acid, 2,6-dichlorophenyl isohexyl ester

Inchi: InChI=1S/C17H22Cl2O4/c1-12(2)6-5-11-22-15(20)9-4-10-16(21)23-17-13(18)7-3-8-14(1
InchiKey: OTHBCYABNYWBIR-UHFFFAOYSA-N
Formula: C17H22Cl2O4
SMILES: CC(C)CCCOC(=O)CCCC(=O)Oc1c(Cl)cccc1Cl
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	2484.00		NIST Webbook
rinpol	2484.00		NIST Webbook
tb	852.00	K	Joback Method
tc	1063.90	K	Joback Method
tf	521.97	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0003039	Pa×s	576.98	Joback Method
dvisc	0.0001945	Pa×s	631.98	Joback Method
dvisc	0.0001337	Pa×s	686.99	Joback Method
dvisc	0.0000971	Pa×s	741.99	Joback Method
dvisc	0.0000738	Pa×s	797.00	Joback Method
dvisc	0.0000580	Pa×s	852.00	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=U358832&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