Dimethylmalonic acid, 2,5-dichlorophenyl isohexyl ester

Inchi: InChI=1S/C17H22Cl2O4/c1-11(2)6-5-9-22-15(20)17(3,4)16(21)23-14-10-12(18)7-8-13(14

InchiKey: WQIFXAIHLRXZFT-UHFFFAOYSA-N

Formula: C17H22Cl2O4

SMILES: CC(C)CCCOC(=O)C(C)(C)C(=O)Oc1cc(Cl)ccc1Cl

Mol. weight [g/mol]: 361.26

Physical Properties

Property code	Value	Unit	Source
gf	-305.89	kJ/mol	Joback Method
hf	-715.73	kJ/mol	Joback Method
hfus	36.08	kJ/mol	Joback Method
hvap	82.43	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.904		Crippen Method
mcvol	265.990	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook
tb	848.77	K	Joback Method
tc	1067.85	K	Joback Method
tf	524.39	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.09	J/mol×K	848.77	Joback Method
cpg	770.43	J/mol×K	885.28	Joback Method
cpg	782.67	J/mol×K	921.80	Joback Method
cpg	793.85	J/mol×K	958.31	Joback Method
cpg	803.99	J/mol×K	994.82	Joback Method
cpg	813.15	J/mol×K	1031.33	Joback Method
cpg	821.36	J/mol×K	1067.85	Joback Method
dvisc	0.0004714	Pa×s	524.39	Joback Method

dvisc	0.0002665	Pa×s	578.45	Joback Method
dvisc	0.0001661	Pa×s	632.52	Joback Method
dvisc	0.0001115	Pa×s	686.58	Joback Method
dvisc	0.0000794	Pa×s	740.64	Joback Method
dvisc	0.0000592	Pa×s	794.71	Joback Method
dvisc	0.0000458	Pa×s	848.77	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=U363682&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