

Dimethylmalonic acid, 2,5-dichlorophenyl isobutyl ester

Inchi:	InChI=1S/C15H18Cl2O4/c1-9(2)8-20-13(18)15(3,4)14(19)21-12-7-10(16)5-6-11(12)17/h5
InchiKey:	HYEIIYZVLIUAIK-UHFFFAOYSA-N
Formula:	C15H18Cl2O4
SMILES:	CC(C)COC(=O)C(C)(C)C(=O)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	333.21

Physical Properties

Property code	Value	Unit	Source
gf	-322.73	kJ/mol	Joback Method
hf	-674.45	kJ/mol	Joback Method
hfus	30.90	kJ/mol	Joback Method
hvap	77.98	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	4.124		Crippen Method
mcvol	237.810	ml/mol	McGowan Method
pc	1870.79	kPa	Joback Method
rinpol	2004.00		NIST Webbook
tb	803.01	K	Joback Method
tc	1026.59	K	Joback Method
tf	501.85	K	Joback Method
vc	0.896	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.84	J/molxK	803.01	Joback Method
cpg	658.69	J/molxK	840.27	Joback Method
cpg	670.48	J/molxK	877.54	Joback Method
cpg	681.25	J/molxK	914.80	Joback Method
cpg	691.01	J/molxK	952.06	Joback Method
cpg	699.82	J/molxK	989.33	Joback Method
cpg	707.70	J/molxK	1026.59	Joback Method
dvisc	0.0005850	Paxs	501.85	Joback Method
dvisc	0.0003390	Paxs	552.04	Joback Method

dvisc	0.0002152	Paxs	602.24	Joback Method
dvisc	0.0001465	Paxs	652.43	Joback Method
dvisc	0.0001053	Paxs	702.62	Joback Method
dvisc	0.0000791	Paxs	752.82	Joback Method
dvisc	0.0000616	Paxs	803.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363679&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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