

Dimethylmalonic acid, 2,4-dichloro-6-formylphenyl propyl ester

Inchi:	InChI=1S/C15H16Cl2O5/c1-4-5-21-13(19)15(2,3)14(20)22-12-9(8-18)6-10(16)7-11(12)17
InchiKey:	HCPCZAZIQYYPNJ-UHFFFAOYSA-N
Formula:	C15H16Cl2O5
SMILES:	CCCOC(=O)C(C)(C)C(=O)Oc1c(Cl)cc(Cl)cc1C=O
Mol. weight [g/mol]:	347.19

Physical Properties

Property code	Value	Unit	Source
gf	-429.44	kJ/mol	Joback Method
hf	-766.22	kJ/mol	Joback Method
hfus	36.32	kJ/mol	Joback Method
hvap	85.75	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.691		Crippen Method
mcvol	239.380	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinpol	2155.00		NIST Webbook
tb	857.09	K	Joback Method
tc	1080.53	K	Joback Method
tf	571.37	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.65	J/molxK	857.09	Joback Method
cpg	664.35	J/molxK	894.33	Joback Method
cpg	674.05	J/molxK	931.57	Joback Method
cpg	682.79	J/molxK	968.81	Joback Method
cpg	690.57	J/molxK	1006.05	Joback Method
cpg	697.44	J/molxK	1043.29	Joback Method
cpg	703.41	J/molxK	1080.53	Joback Method
dvisc	0.0004449	Paxs	571.37	Joback Method
dvisc	0.0002925	Paxs	618.99	Joback Method

dvisc	0.0002042	Paxs	666.61	Joback Method
dvisc	0.0001495	Paxs	714.23	Joback Method
dvisc	0.0001139	Paxs	761.85	Joback Method
dvisc	0.0000895	Paxs	809.47	Joback Method
dvisc	0.0000723	Paxs	857.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363630&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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