

Dimethylmalonic acid, propyl 2,3,5-trichlorophenyl ester

Inchi:	InChI=1S/C14H15Cl3O4/c1-4-5-20-12(18)14(2,3)13(19)21-10-7-8(15)6-9(16)11(10)17/h6
InchiKey:	PEGMVXZLURBLDL-UHFFFAOYSA-N
Formula:	C14H15Cl3O4
SMILES:	CCCOC(=O)C(C)(C)C(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	353.62

Physical Properties

Property code	Value	Unit	Source
gf	-350.27	kJ/mol	Joback Method
hf	-675.74	kJ/mol	Joback Method
hfus	35.64	kJ/mol	Joback Method
hvap	81.19	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.532		Crippen Method
mvol	235.960	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	2143.00		NIST Webbook
tb	822.98	K	Joback Method
tc	1049.66	K	Joback Method
tf	548.02	K	Joback Method
vc	0.895	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.60	J/molxK	822.98	Joback Method
cpg	657.48	J/molxK	1011.88	Joback Method
cpg	650.15	J/molxK	974.10	Joback Method
cpg	641.93	J/molxK	936.32	Joback Method
cpg	632.78	J/molxK	898.54	Joback Method
cpg	622.67	J/molxK	860.76	Joback Method
cpg	663.93	J/molxK	1049.66	Joback Method
dvisc	0.0000672	Paxs	822.98	Joback Method
dvisc	0.0000834	Paxs	777.15	Joback Method

dvisc	0.0001062	Paxs	731.33	Joback Method
dvisc	0.0001397	Paxs	685.50	Joback Method
dvisc	0.0001911	Paxs	639.67	Joback Method
dvisc	0.0002744	Paxs	593.85	Joback Method
dvisc	0.0004186	Paxs	548.02	Joback Method

Sources

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=U363905&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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