

Diethylmalonic acid, monochloride, 2-acetylphenyl ester

Inchi:	InChI=1S/C15H17ClO4/c1-4-15(5-2,13(16)18)14(19)20-12-9-7-6-8-11(12)10(3)17/h6-9H,
InchiKey:	FBKCCGFEXILLV-UHFFFAOYSA-N
Formula:	C15H17ClO4
SMILES:	CCC(CC)(C(=O)Cl)C(=O)Oc1ccccc1C(C)=O
Mol. weight [g/mol]:	296.75

Physical Properties

Property code	Value	Unit	Source
gf	-322.65	kJ/mol	Joback Method
hf	-622.32	kJ/mol	Joback Method
hfus	31.03	kJ/mol	Joback Method
hvap	77.66	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.366		Crippen Method
mcvol	221.270	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinsol	1969.00		NIST Webbook
tb	792.49	K	Joback Method
tc	1016.59	K	Joback Method
tf	502.11	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.02	J/molxK	792.49	Joback Method
cpg	621.63	J/molxK	829.84	Joback Method
cpg	633.21	J/molxK	867.19	Joback Method
cpg	643.83	J/molxK	904.54	Joback Method
cpg	653.53	J/molxK	941.89	Joback Method
cpg	662.37	J/molxK	979.24	Joback Method
cpg	670.39	J/molxK	1016.59	Joback Method
dvisc	0.0008578	Paxs	502.11	Joback Method
dvisc	0.0005093	Paxs	550.51	Joback Method

dvisc	0.0003290	Paxs	598.90	Joback Method
dvisc	0.0002269	Paxs	647.30	Joback Method
dvisc	0.0001647	Paxs	695.70	Joback Method
dvisc	0.0001247	Paxs	744.09	Joback Method
dvisc	0.0000977	Paxs	792.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370103&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
mvol:	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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