

Diethylmalonic acid, monochloride, 3-phenylpropyl ester

Inchi:	InChI=1S/C16H21ClO3/c1-3-16(4-2,14(17)18)15(19)20-12-8-11-13-9-6-5-7-10-13/h5-7,9
InchiKey:	AZTXEHGYZXHJY-UHFFFAOYSA-N
Formula:	C16H21ClO3
SMILES:	CCC(CC)(C(=O)Cl)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	296.79

Physical Properties

Property code	Value	Unit	Source
gf	-175.68	kJ/mol	Joback Method
hf	-518.91	kJ/mol	Joback Method
hfus	32.41	kJ/mol	Joback Method
hvap	72.48	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.734		Crippen Method
mvol	233.790	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
rinpol	1971.00		NIST Webbook
tb	756.52	K	Joback Method
tc	971.17	K	Joback Method
tf	450.93	K	Joback Method
vc	0.891	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.99	J/molxK	756.52	Joback Method
cpg	665.79	J/molxK	792.30	Joback Method
cpg	679.53	J/molxK	828.07	Joback Method
cpg	692.26	J/molxK	863.85	Joback Method
cpg	704.04	J/molxK	899.62	Joback Method
cpg	714.93	J/molxK	935.40	Joback Method
cpg	724.99	J/molxK	971.17	Joback Method
dvisc	0.0011669	Paxs	450.93	Joback Method
dvisc	0.0006108	Paxs	501.86	Joback Method

dvisc	0.0003602	Paxs	552.79	Joback Method
dvisc	0.0002322	Paxs	603.73	Joback Method
dvisc	0.0001603	Paxs	654.66	Joback Method
dvisc	0.0001167	Paxs	705.59	Joback Method
dvisc	0.0000887	Paxs	756.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369669&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

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