

Diethylmalonic acid, monochloride, 2-isopropoxyphenyl ester

Inchi:	InChI=1S/C16H21ClO4/c1-5-16(6-2,14(17)18)15(19)21-13-10-8-7-9-12(13)20-11(3)4/h7-
InchiKey:	ASUNEVXLSQBBSM-UHFFFAOYSA-N
Formula:	C16H21ClO4
SMILES:	CCC(CC)(C(=O)Cl)C(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]:	312.79

Physical Properties

Property code	Value	Unit	Source
gf	-292.75	kJ/mol	Joback Method
hf	-667.88	kJ/mol	Joback Method
hfus	29.68	kJ/mol	Joback Method
hvap	75.16	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.951		Crippen Method
mcvol	239.660	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinsol	1938.00		NIST Webbook
tb	783.48	K	Joback Method
tc	1000.54	K	Joback Method
tf	470.68	K	Joback Method
vc	0.903	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.63	J/molxK	783.48	Joback Method
cpg	692.10	J/molxK	819.66	Joback Method
cpg	705.47	J/molxK	855.83	Joback Method
cpg	717.77	J/molxK	892.01	Joback Method
cpg	729.04	J/molxK	928.18	Joback Method
cpg	739.33	J/molxK	964.36	Joback Method
cpg	748.66	J/molxK	1000.54	Joback Method
dvisc	0.0007742	Paxs	470.68	Joback Method
dvisc	0.0004113	Paxs	522.81	Joback Method

dvisc	0.0002451	Paxs	574.95	Joback Method
dvisc	0.0001592	Paxs	627.08	Joback Method
dvisc	0.0001104	Paxs	679.21	Joback Method
dvisc	0.0000807	Paxs	731.35	Joback Method
dvisc	0.0000615	Paxs	783.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369597&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

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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