Diethylmalonic acid, monochloride, 2-isopropylphenyl ester

Inchi: InChI=1S/C16H21ClO3/c1-5-16(6-2,14(17)18)15(19)20-13-10-8-7-9-12(13)11(3)4/h7-11H

InchiKey: NTKDZOOGHVEBRW-UHFFFAOYSA-N

Formula: C16H21ClO3

SMILES: CCC(CC)(C(=O)Cl)C(=O)Oc1ccccc1C(C)C

Mol. weight [g/mol]: 296.79

Physical Properties

Property code	Value	Unit	Source
gf	-187.75	kJ/mol	Joback Method
hf	-535.66	kJ/mol	Joback Method
hfus	28.49	kJ/mol	Joback Method
hvap	72.75	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.287		Crippen Method
mcvol	233.790	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	1827.00		NIST Webbook
rinpol	1827.00		NIST Webbook
tb	761.06	K	Joback Method
tc	979.98	K	Joback Method
tf	448.45	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.56	J/mol×K	761.06	Joback Method
cpg	714.86	J/mol×K	943.50	Joback Method
cpg	703.96	J/mol×K	907.01	Joback Method
cpg	692.14	J/mol×K	870.52	Joback Method
cpg	679.33	J/mol×K	834.03	Joback Method
cpg	665.49	J/mol×K	797.55	Joback Method
cpg	724.88	J/mol×K	979.98	Joback Method
dvisc	0.0000818	Pa×s	761.06	Joback Method

dvisc	0.0001079	Pa×s	708.96	Joback Method
dvisc	0.0001487	Pa×s	656.86	Joback Method
dvisc	0.0002164	Pa×s	604.75	Joback Method
dvisc	0.0003382	Pa×s	552.65	Joback Method
dvisc	0.0005799	Pa×s	500.55	Joback Method
dvisc	0.0011272	Pa×s	448.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369985&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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