Diethylmalonic acid, monochloride, 1-phenylpropyl ester

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

InchiKey: ZXWZQVWUEBQBKK-UHFFFAOYSA-N

Formula: C16H21ClO3

SMILES: CCC(OC(=O)C(CC)(CC)C(=O)Cl)c1ccccc1

Mol. weight [g/mol]: 296.79

Physical Properties

Property code	Value	Unit	Source
gf	-178.12	kJ/mol	Joback Method
hf	-524.19	kJ/mol	Joback Method
hfus	28.88	kJ/mol	Joback Method
hvap	72.09	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.253		Crippen Method
mcvol	233.790	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	1813.00		NIST Webbook
rinpol	1813.00		NIST Webbook
tb	756.08	K	Joback Method
tc	974.23	K	Joback Method
tf	435.93	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.55	J/mol×K	756.08	Joback Method
cpg	716.29	J/mol×K	937.87	Joback Method
cpg	705.32	J/mol×K	901.51	Joback Method
cpg	693.42	J/mol×K	865.15	Joback Method
cpg	680.54	J/mol×K	828.80	Joback Method
cpg	666.60	J/mol×K	792.44	Joback Method
cpg	726.40	J/mol×K	974.23	Joback Method
dvisc	0.0000817	Pa×s	756.08	Joback Method

dvisc	0.0001095	Pa×s	702.72	Joback Method
dvisc	0.0001540	Pa×s	649.36	Joback Method
dvisc	0.0002301	Pa×s	596.01	Joback Method
dvisc	0.0003723	Pa×s	542.65	Joback Method
dvisc	0.0006687	Pa×s	489.29	Joback Method
dvisc	0.0013863	Pa×s	435.93	Joback Method

Sources

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=U370193&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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