

Diethylmalonic acid, 4-chloro-3-methylphenyl ethyl ester

Inchi:	InChI=1S/C16H21ClO4/c1-5-16(6-2,14(18)20-7-3)15(19)21-12-8-9-13(17)11(4)10-12/h8-
InchiKey:	RBSUHTKVPBQRHK-UHFFFAOYSA-N
Formula:	C16H21ClO4
SMILES:	CCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	312.79

Physical Properties

Property code	Value	Unit	Source
gf	-299.94	kJ/mol	Joback Method
hf	-674.07	kJ/mol	Joback Method
hfus	32.82	kJ/mol	Joback Method
hvap	76.21	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.923		Crippen Method
mcvol	239.660	ml/mol	McGowan Method
pc	1766.90	kPa	Joback Method
rinpol	1978.00		NIST Webbook
rinpol	1978.00		NIST Webbook
tb	788.90	K	Joback Method
tc	1003.50	K	Joback Method
tf	498.20	K	Joback Method
vc	0.909	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.00	J/molxK	788.90	Joback Method
cpg	690.15	J/molxK	824.67	Joback Method
cpg	703.26	J/molxK	860.43	Joback Method
cpg	715.35	J/molxK	896.20	Joback Method
cpg	726.45	J/molxK	931.97	Joback Method
cpg	736.60	J/molxK	967.74	Joback Method
cpg	745.82	J/molxK	1003.50	Joback Method
dvisc	0.0005728	Paxs	498.20	Joback Method

dvisc	0.0003422	Paxs	546.65	Joback Method
dvisc	0.0002223	Paxs	595.10	Joback Method
dvisc	0.0001541	Paxs	643.55	Joback Method
dvisc	0.0001124	Paxs	692.00	Joback Method
dvisc	0.0000855	Paxs	740.45	Joback Method
dvisc	0.0000672	Paxs	788.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369910&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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