

Diethylmalonic acid, 2-chloro-5-methylphenyl octyl ester

Inchi:	InChI=1S/C22H33ClO4/c1-5-8-9-10-11-12-15-26-20(24)22(6-2,7-3)21(25)27-19-16-17(4)
InchiKey:	UQWLVXXPANUXOT-UHFFFAOYSA-N
Formula:	C22H33ClO4
SMILES:	CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(C)ccc1Cl
Mol. weight [g/mol]:	396.95

Physical Properties

Property code	Value	Unit	Source
gf	-249.42	kJ/mol	Joback Method
hf	-797.91	kJ/mol	Joback Method
hfus	48.36	kJ/mol	Joback Method
hvap	89.57	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	6.264		Crippen Method
mcvol	324.200	ml/mol	McGowan Method
pc	1145.21	kPa	Joback Method
rinpol	2527.00		NIST Webbook
rinpol	2527.00		NIST Webbook
tb	926.18	K	Joback Method
tc	1139.21	K	Joback Method
tf	565.82	K	Joback Method
vc	1.246	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1023.93	J/molxK	926.18	Joback Method
cpg	1039.29	J/molxK	961.69	Joback Method
cpg	1053.43	J/molxK	997.19	Joback Method
cpg	1066.40	J/molxK	1032.70	Joback Method
cpg	1078.24	J/molxK	1068.20	Joback Method
cpg	1089.00	J/molxK	1103.71	Joback Method
cpg	1098.73	J/molxK	1139.21	Joback Method
dvisc	0.0002985	Paxs	565.82	Joback Method

dvisc	0.0001659	Paxs	625.88	Joback Method
dvisc	0.0001022	Paxs	685.94	Joback Method
dvisc	0.0000681	Paxs	746.00	Joback Method
dvisc	0.0000482	Paxs	806.06	Joback Method
dvisc	0.0000358	Paxs	866.12	Joback Method
dvisc	0.0000276	Paxs	926.18	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=U370458&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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