

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

Inchi:	InChI=1S/C25H39ClO4/c1-5-8-9-10-11-12-13-14-15-18-29-23(27)25(6-2,7-3)24(28)30-2
InchiKey:	PEOGCBIPLSUMDX-UHFFFAOYSA-N
Formula:	C25H39ClO4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	439.03

Physical Properties

Property code	Value	Unit	Source
gf	-224.16	kJ/mol	Joback Method
hf	-859.83	kJ/mol	Joback Method
hfus	56.13	kJ/mol	Joback Method
hvap	96.24	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	7.434		Crippen Method
mvol	366.470	ml/mol	McGowan Method
pc	950.84	kPa	Joback Method
rinpol	2827.00		NIST Webbook
rinpol	2827.00		NIST Webbook
tb	994.82	K	Joback Method
tc	1217.98	K	Joback Method
tf	599.63	K	Joback Method
vc	1.413	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1206.95	J/molxK	994.82	Joback Method
cpg	1273.91	J/molxK	1180.78	Joback Method
cpg	1263.02	J/molxK	1143.59	Joback Method
cpg	1250.94	J/molxK	1106.40	Joback Method
cpg	1237.62	J/molxK	1069.21	Joback Method
cpg	1222.98	J/molxK	1032.01	Joback Method
cpg	1283.68	J/molxK	1217.98	Joback Method
dvisc	0.0000173	Paxs	994.82	Joback Method

dvisc	0.0000225	Paxs	928.95	Joback Method
dvisc	0.0000307	Paxs	863.09	Joback Method
dvisc	0.0000439	Paxs	797.23	Joback Method
dvisc	0.0000670	Paxs	731.36	Joback Method
dvisc	0.0001111	Paxs	665.50	Joback Method
dvisc	0.0002061	Paxs	599.63	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369920&Units=SI

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
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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