

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

Inchi:	InChI=1S/C26H41ClO4/c1-5-8-9-10-11-12-13-14-15-16-19-30-24(28)26(6-2,7-3)25(29)3
InchiKey:	LPBPRHWFFBWPLY-UHFFFAOYSA-N
Formula:	C26H41ClO4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(C)ccc1Cl
Mol. weight [g/mol]:	453.05

Physical Properties

Property code	Value	Unit	Source
gf	-215.74	kJ/mol	Joback Method
hf	-880.47	kJ/mol	Joback Method
hfus	58.72	kJ/mol	Joback Method
hvap	98.47	kJ/mol	Joback Method
log10ws	-8.68		Crippen Method
logp	7.824		Crippen Method
mvol	380.560	ml/mol	McGowan Method
pc	896.95	kPa	Joback Method
rinpol	2944.00		NIST Webbook
rinpol	2944.00		NIST Webbook
tb	1017.70	K	Joback Method
tc	1246.25	K	Joback Method
tf	610.90	K	Joback Method
vc	1.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1268.95	J/molxK	1017.70	Joback Method
cpg	1285.25	J/molxK	1055.79	Joback Method
cpg	1300.09	J/molxK	1093.88	Joback Method
cpg	1313.56	J/molxK	1131.97	Joback Method
cpg	1325.72	J/molxK	1170.06	Joback Method
cpg	1336.65	J/molxK	1208.15	Joback Method
cpg	1346.43	J/molxK	1246.25	Joback Method
dvisc	0.0001813	Paxs	610.90	Joback Method

dvisc	0.0000968	Paxs	678.70	Joback Method
dvisc	0.0000579	Paxs	746.50	Joback Method
dvisc	0.0000377	Paxs	814.30	Joback Method
dvisc	0.0000263	Paxs	882.10	Joback Method
dvisc	0.0000193	Paxs	949.90	Joback Method
dvisc	0.0000147	Paxs	1017.70	Joback Method

Sources

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=U370461&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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