

Diethylmalonic acid, 2,3-dichlorophenyl tridecyl ester

Inchi:	InChI=1S/C26H40Cl2O4/c1-4-7-8-9-10-11-12-13-14-15-16-20-31-24(29)26(5-2,6-3)25(30)
InchiKey:	CIFKZBWIZCZYSB-UHFFFAOYSA-N
Formula:	C26H40Cl2O4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	487.50

Physical Properties

Property code	Value	Unit	Source
gf	-227.67	kJ/mol	Joback Method
hf	-896.21	kJ/mol	Joback Method
hfus	62.91	kJ/mol	Joback Method
hvap	102.86	kJ/mol	Joback Method
log10ws	-9.31		Crippen Method
logp	8.559		Crippen Method
mvol	392.800	ml/mol	McGowan Method
pc	877.39	kPa	Joback Method
rinpol	3140.00		NIST Webbook
rinpol	3140.00		NIST Webbook
tb	1055.13	K	Joback Method
tc	1293.12	K	Joback Method
tf	640.82	K	Joback Method
vc	1.518	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1292.89	J/molxK	1055.13	Joback Method
cpg	1355.23	J/molxK	1253.46	Joback Method
cpg	1345.33	J/molxK	1213.79	Joback Method
cpg	1334.24	J/molxK	1174.13	Joback Method
cpg	1321.86	J/molxK	1134.46	Joback Method
cpg	1308.11	J/molxK	1094.80	Joback Method
cpg	1364.01	J/molxK	1293.12	Joback Method
dvisc	0.0000121	Paxs	1055.13	Joback Method

dvisc	0.0000158	Paxs	986.08	Joback Method
dvisc	0.0000215	Paxs	917.03	Joback Method
dvisc	0.0000307	Paxs	847.97	Joback Method
dvisc	0.0000467	Paxs	778.92	Joback Method
dvisc	0.0000771	Paxs	709.87	Joback Method
dvisc	0.0001416	Paxs	640.82	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=U370041&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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