

Dimethylmalonic acid, 4-chlorophenyl hexadecyl ester

Inchi: InChI=1S/C27H43ClO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-31-25(29)27(2,3)26
InchiKey: ZWPCRXXMASOHPN-UHFFFAOYSA-N
Formula: C27H43ClO4
SMILES: CCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 467.08

Physical Properties

Property code	Value	Unit	Source
gf	-197.69	kJ/mol	Joback Method
hf	-889.64	kJ/mol	Joback Method
hfus	61.69	kJ/mol	Joback Method
hvap	100.03	kJ/mol	Joback Method
log10ws	-9.04		Crippen Method
logp	8.296		Crippen Method
mcvol	394.650	ml/mol	McGowan Method
pc	854.96	kPa	Joback Method
rinpol	3105.00		NIST Webbook
rinpol	3105.00		NIST Webbook
tb	1035.60	K	Joback Method
tc	1269.41	K	Joback Method
tf	609.65	K	Joback Method
vc	1.526	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1332.20	J/molxK	1035.60	Joback Method
cpg	1348.97	J/molxK	1074.57	Joback Method
cpg	1364.25	J/molxK	1113.54	Joback Method
cpg	1378.13	J/molxK	1152.50	Joback Method
cpg	1390.71	J/molxK	1191.47	Joback Method
cpg	1402.08	J/molxK	1230.44	Joback Method
cpg	1412.33	J/molxK	1269.41	Joback Method
dvisc	0.0001793	Paxs	609.65	Joback Method

dvisc	0.0000907	Paxs	680.64	Joback Method
dvisc	0.0000522	Paxs	751.63	Joback Method
dvisc	0.0000330	Paxs	822.62	Joback Method
dvisc	0.0000225	Paxs	893.62	Joback Method
dvisc	0.0000162	Paxs	964.61	Joback Method
dvisc	0.0000122	Paxs	1035.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361984&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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

Latest version available from:

<https://www.chemeo.com/cid/94-780-2/Dimethylmalonic-acid-4-chlorophenyl-hexadecyl-ester.pdf>

Generated by Cheméo on 2024-04-23 16:32:52.692960168 +0000 UTC m=+16179221.613537483.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.