

Diethylmalonic acid, 3-methylbenzyl undecyl ester

Inchi:	InChI=1S/C26H42O4/c1-5-8-9-10-11-12-13-14-15-19-29-24(27)26(6-2,7-3)25(28)30-21-2
InchiKey:	ZOAGZCRGCSQXHO-UHFFFAOYSA-N
Formula:	C26H42O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(C)c1
Mol. weight [g/mol]:	418.61

Physical Properties

Property code	Value	Unit	Source
gf	-194.18	kJ/mol	Joback Method
hf	-853.26	kJ/mol	Joback Method
hfus	54.91	kJ/mol	Joback Method
hvap	93.42	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	6.919		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	925.55	kPa	Joback Method
rinsol	2748.00		NIST Webbook
tb	975.29	K	Joback Method
tc	1194.04	K	Joback Method
tf	568.46	K	Joback Method
vc	1.421	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1243.60	J/molxK	975.29	Joback Method
cpg	1317.86	J/molxK	1157.58	Joback Method
cpg	1305.54	J/molxK	1121.12	Joback Method
cpg	1292.02	J/molxK	1084.66	Joback Method
cpg	1277.24	J/molxK	1048.21	Joback Method
cpg	1261.12	J/molxK	1011.75	Joback Method
cpg	1329.05	J/molxK	1194.04	Joback Method
dvisc	0.0000173	Paxs	975.29	Joback Method
dvisc	0.0000230	Paxs	907.49	Joback Method

dvisc	0.0000320	Paxs	839.68	Joback Method
dvisc	0.0000472	Paxs	771.88	Joback Method
dvisc	0.0000751	Paxs	704.07	Joback Method
dvisc	0.0001319	Paxs	636.26	Joback Method
dvisc	0.0002647	Paxs	568.46	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=U369312&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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