

Diethylmalonic acid, phenethyl undecyl ester

Inchi:	InChI=1S/C26H42O4/c1-4-7-8-9-10-11-12-13-17-21-29-24(27)26(5-2,6-3)25(28)30-22-20
InchiKey:	SISFRWACTASMEU-UHFFFAOYSA-N
Formula:	C26H42O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	418.61

Physical Properties

Property code	Value	Unit	Source
gf	-184.55	kJ/mol	Joback Method
hf	-841.79	kJ/mol	Joback Method
hfus	55.30	kJ/mol	Joback Method
hvap	92.76	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	6.653		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	934.06	kPa	Joback Method
rinpol	2743.00		NIST Webbook
tb	970.31	K	Joback Method
tc	1187.95	K	Joback Method
tf	555.94	K	Joback Method
vc	1.421	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1244.13	J/molxK	970.31	Joback Method
cpg	1319.26	J/molxK	1151.68	Joback Method
cpg	1306.69	J/molxK	1115.41	Joback Method
cpg	1292.97	J/molxK	1079.13	Joback Method
cpg	1278.02	J/molxK	1042.86	Joback Method
cpg	1261.77	J/molxK	1006.58	Joback Method
cpg	1330.75	J/molxK	1187.95	Joback Method
dvisc	0.0000169	Paxs	970.31	Joback Method
dvisc	0.0000228	Paxs	901.25	Joback Method

dvisc	0.0000323	Paxs	832.19	Joback Method
dvisc	0.0000486	Paxs	763.12	Joback Method
dvisc	0.0000794	Paxs	694.06	Joback Method
dvisc	0.0001448	Paxs	625.00	Joback Method
dvisc	0.0003062	Paxs	555.94	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=U369554&Units=SI

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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