

Diethylmalonic acid, dodecyl phenethyl ester

Inchi:	InChI=1S/C27H44O4/c1-4-7-8-9-10-11-12-13-14-18-22-30-25(28)27(5-2,6-3)26(29)31-23
InchiKey:	UJSGOURYJZEQEP-UHFFFAOYSA-N
Formula:	C27H44O4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	432.64

Physical Properties

Property code	Value	Unit	Source
gf	-176.13	kJ/mol	Joback Method
hf	-862.43	kJ/mol	Joback Method
hfus	57.89	kJ/mol	Joback Method
hvap	94.99	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	7.043		Crippen Method
mvol	382.410	ml/mol	McGowan Method
pc	881.57	kPa	Joback Method
rinpol	2847.00		NIST Webbook
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tb	993.19	K	Joback Method
tc	1216.27	K	Joback Method
tf	567.21	K	Joback Method
vc	1.476	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1306.86	J/molxK	993.19	Joback Method
cpg	1324.82	J/molxK	1030.37	Joback Method
cpg	1341.33	J/molxK	1067.55	Joback Method
cpg	1356.47	J/molxK	1104.73	Joback Method
cpg	1370.34	J/molxK	1141.91	Joback Method
cpg	1383.02	J/molxK	1179.09	Joback Method
cpg	1394.60	J/molxK	1216.27	Joback Method
dvisc	0.0002676	Paxs	567.21	Joback Method

dvisc	0.0001254	Paxs	638.21	Joback Method
dvisc	0.0000684	Paxs	709.20	Joback Method
dvisc	0.0000417	Paxs	780.20	Joback Method
dvisc	0.0000276	Paxs	851.20	Joback Method
dvisc	0.0000194	Paxs	922.19	Joback Method
dvisc	0.0000144	Paxs	993.19	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=U369555&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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