Diethylmalonic acid, 3-phenylpropyl undecyl ester

Inchi: InChI=1S/C27H44O4/c1-4-7-8-9-10-11-12-13-17-22-30-25(28)27(5-2,6-3)26(29)31-23-18
InchiKey: QJJIUPSAEKIOPX-UHFFFAOYSA-N
Formula: C27H44O4
SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCc1ccccc1
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
mcvol	382.410	ml/mol	McGowan Method
pc	881.57	kPa	Joback Method
rinpol	2887.00		NIST Webbook
tb	993.19	K	Joback Method
tc	1216.27	K	Joback Method
tf	567.21	K	Joback Method
vc	1.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1306.86	J/mol×K	993.19	Joback Method
cpg	1324.82	J/mol×K	1030.37	Joback Method
cpg	1341.33	J/mol×K	1067.55	Joback Method
cpg	1356.47	J/mol×K	1104.73	Joback Method
cpg	1370.34	J/mol×K	1141.91	Joback Method
cpg	1383.02	J/mol×K	1179.09	Joback Method
cpg	1394.60	J/mol×K	1216.27	Joback Method
dvisc	0.0002676	Pa×s	567.21	Joback Method
dvisc	0.0001254	Pa×s	638.21	Joback Method

dvisc	0.0000684	Pa×s	709.20	Joback Method
dvisc	0.0000417	Pa×s	780.20	Joback Method
dvisc	0.0000276	Pa×s	851.20	Joback Method
dvisc	0.0000194	Pa×s	922.19	Joback Method
dvisc	0.0000144	Pa×s	993.19	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=U369661&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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