

Dimethylmalonic acid, pentadecyl 2-phenethyl ester

Inchi:	InChI=1S/C28H46O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-19-23-31-26(29)28(2,3)27(30)32
InchiKey:	XYEZXYLEUNCHJA-UHFFFAOYSA-N
Formula:	C28H46O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	446.66

Physical Properties

Property code	Value	Unit	Source
gf	-167.71	kJ/mol	Joback Method
hf	-883.07	kJ/mol	Joback Method
hfus	60.48	kJ/mol	Joback Method
hvap	97.21	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	7.433		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	833.38	kPa	Joback Method
rinpol	3033.00		NIST Webbook
tb	1016.07	K	Joback Method
tc	1245.70	K	Joback Method
tf	578.48	K	Joback Method
vc	1.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1370.03	J/molxK	1016.07	Joback Method
cpg	1447.37	J/molxK	1207.43	Joback Method
cpg	1434.56	J/molxK	1169.15	Joback Method
cpg	1420.52	J/molxK	1130.88	Joback Method
cpg	1405.15	J/molxK	1092.61	Joback Method
cpg	1388.35	J/molxK	1054.34	Joback Method
cpg	1459.06	J/molxK	1245.70	Joback Method
dvisc	0.0000123	Paxs	1016.07	Joback Method
dvisc	0.0000166	Paxs	943.14	Joback Method

dvisc	0.0000235	Paxs	870.21	Joback Method
dvisc	0.0000357	Paxs	797.27	Joback Method
dvisc	0.0000588	Paxs	724.34	Joback Method
dvisc	0.0001085	Paxs	651.41	Joback Method
dvisc	0.0002333	Paxs	578.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361625&Units=SI
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

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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