

Diethylmalonic acid, 2-formylphenyl tetradecyl ester

Inchi: InChI=1S/C28H44O5/c1-4-7-8-9-10-11-12-13-14-15-16-19-22-32-26(30)28(5-2,6-3)27(31)
InchiKey: LORJISMCQZIGHO-UHFFFAOYSA-N
Formula: C28H44O5
SMILES: CCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1C=O
Mol. weight [g/mol]: 460.65

Physical Properties

Property code	Value	Unit	Source
gf	-276.86	kJ/mol	Joback Method
hf	-980.12	kJ/mol	Joback Method
hfus	62.38	kJ/mol	Joback Method
hvap	104.60	kJ/mol	Joback Method
log10ws	-8.60		Crippen Method
logp	7.455		Crippen Method
mcvol	398.070	ml/mol	McGowan Method
pc	862.51	kPa	Joback Method
rinpol	3178.00		NIST Webbook
tb	1069.71	K	Joback Method
tc	1315.21	K	Joback Method
tf	633.00	K	Joback Method
vc	1.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1381.72	J/mol×K	1069.71	Joback Method
cpg	1398.19	J/mol×K	1110.63	Joback Method
cpg	1413.03	J/mol×K	1151.54	Joback Method
cpg	1426.34	J/mol×K	1192.46	Joback Method
cpg	1438.25	J/mol×K	1233.38	Joback Method
cpg	1448.85	J/mol×K	1274.29	Joback Method
cpg	1458.25	J/mol×K	1315.21	Joback Method
dvisc	0.0001844	Pa×s	633.00	Joback Method
dvisc	0.0000946	Pa×s	705.78	Joback Method

dvisc	0.0000550	Pa×s	778.57	Joback Method
dvisc	0.0000350	Pa×s	851.36	Joback Method
dvisc	0.0000240	Pa×s	924.14	Joback Method
dvisc	0.0000174	Pa×s	996.93	Joback Method
dvisc	0.0000131	Pa×s	1069.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369959&Units=SI
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

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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