

Dimethylmalonic acid, decyl 4-(4-methoxyphenyl)cyclohexyl ester

Inchi: InChI=1S/C28H44O5/c1-5-6-7-8-9-10-11-12-21-32-26(29)28(2,3)27(30)33-25-19-15-23(1)
InchiKey: FARJRDIZHIVRNG-UHFFFAOYSA-N
Formula: C28H44O5
SMILES: CCCCCCCCCCOC(=O)C(C)(C)C(=O)OC1CCC(c2ccc(OC)cc2)CC1
Mol. weight [g/mol]: 460.65

Physical Properties

Property code	Value	Unit	Source
gf	-265.60	kJ/mol	Joback Method
hf	-992.78	kJ/mol	Joback Method
hfus	54.18	kJ/mol	Joback Method
hvap	100.41	kJ/mol	Joback Method
log10ws	-7.80		Crippen Method
logp	6.975		Crippen Method
mcvol	391.510	ml/mol	McGowan Method
pc	905.06	kPa	Joback Method
rinpol	3398.00		NIST Webbook
rinpol	3398.00		NIST Webbook
tb	1058.35	K	Joback Method
tc	1295.73	K	Joback Method
tf	616.37	K	Joback Method
vc	1.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1395.87	J/mol×K	1058.35	Joback Method
cpg	1411.42	J/mol×K	1097.91	Joback Method
cpg	1424.92	J/mol×K	1137.48	Joback Method
cpg	1436.45	J/mol×K	1177.04	Joback Method
cpg	1446.08	J/mol×K	1216.60	Joback Method
cpg	1453.88	J/mol×K	1256.17	Joback Method
cpg	1459.92	J/mol×K	1295.73	Joback Method
dvisc	0.0001794	Pa×s	616.37	Joback Method

dvisc	0.0000912	Pa×s	690.03	Joback Method
dvisc	0.0000528	Pa×s	763.70	Joback Method
dvisc	0.0000337	Pa×s	837.36	Joback Method
dvisc	0.0000231	Pa×s	911.02	Joback Method
dvisc	0.0000168	Pa×s	984.69	Joback Method
dvisc	0.0000127	Pa×s	1058.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363922&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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