

Dimethylmalonic acid, hexadecyl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C30H50O5/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-21-24-33-28(31)30(4,5)29
InchiKey: VRMQUQNACGGLIQ-UHFFFAOYSA-N
Formula: C30H50O5
SMILES: CCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]: 490.71

Physical Properties

Property code	Value	Unit	Source
gf	-267.94	kJ/mol	Joback Method
hf	-1073.32	kJ/mol	Joback Method
hfus	62.93	kJ/mol	Joback Method
hvap	104.35	kJ/mol	Joback Method
log10ws	-9.43		Crippen Method
logp	8.430		Crippen Method
mvol	430.550	ml/mol	McGowan Method
pc	738.42	kPa	Joback Method
rinpol	3174.00		NIST Webbook
rinpol	3174.00		NIST Webbook
tb	1088.79	K	Joback Method
tc	1344.16	K	Joback Method
tf	620.77	K	Joback Method
vc	1.657	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1525.07	J/molxK	1088.79	Joback Method
cpg	1593.43	J/molxK	1301.60	Joback Method
cpg	1583.51	J/molxK	1259.04	Joback Method
cpg	1571.83	J/molxK	1216.47	Joback Method
cpg	1558.26	J/molxK	1173.91	Joback Method
cpg	1542.71	J/molxK	1131.35	Joback Method
cpg	1601.69	J/molxK	1344.16	Joback Method
dvisc	0.0000060	Paxs	1088.79	Joback Method

dvisc	0.0000081	Paxs	1010.79	Joback Method
dvisc	0.0000115	Paxs	932.78	Joback Method
dvisc	0.0000174	Paxs	854.78	Joback Method
dvisc	0.0000287	Paxs	776.78	Joback Method
dvisc	0.0000530	Paxs	698.77	Joback Method
dvisc	0.0001138	Paxs	620.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361864&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

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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