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

Inchi: InChI=1S/C27H42O5/c1-5-6-7-8-9-10-11-20-31-25(28)27(2,3)26(29)32-24-18-14-22(15-1

InchiKey: ISIYULXCEQSXKG-UHFFFAOYSA-N

Formula: C27H42O5

SMILES: CCCCCCCCCOC(=O)C(C)(C)C(=O)OC1CCC(c2ccc(OC)cc2)CC1

Mol. weight [g/mol]: 446.62

Physical Properties

Property code	Value	Unit	Source
gf	-274.02	kJ/mol	Joback Method
hf	-972.14	kJ/mol	Joback Method
hfus	51.59	kJ/mol	Joback Method
hvap	98.18	kJ/mol	Joback Method
log10ws	-7.38		Crippen Method
logp	6.585		Crippen Method
mcvol	377.420	ml/mol	McGowan Method
pc	959.69	kPa	Joback Method
rinpol	3303.00		NIST Webbook
tb	1035.47	K	Joback Method
tc	1268.10	K	Joback Method
tf	605.10	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1333.57	J/mol×K	1035.47	Joback Method
cpg	1393.01	J/mol×K	1229.33	Joback Method
cpg	1384.79	J/mol×K	1190.56	Joback Method
cpg	1374.79	J/mol×K	1151.79	Joback Method
cpg	1362.97	J/mol×K	1113.01	Joback Method
cpg	1349.25	J/mol×K	1074.24	Joback Method
cpg	1399.54	J/mol×K	1268.10	Joback Method
dvisc	0.0000149	Pa×s	1035.47	Joback Method
dvisc	0.0000196	Pa×s	963.74	Joback Method

dvisc	0.0000270	Pa×s	892.01	Joback Method
dvisc	0.0000392	Pa×s	820.28	Joback Method
dvisc	0.0000611	Pa×s	748.56	Joback Method
dvisc	0.0001048	Pa×s	676.83	Joback Method
dvisc	0.0002044	Pa×s	605.10	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=U363921&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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