

Dimethylmalonic acid, octadecyl 2-phenethyl ester

Inchi:	InChI=1S/C31H52O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-26-34-29(32)31(2,3
InchiKey:	YGQJUAQHSNZMJN-UHFFFAOYSA-N
Formula:	C31H52O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	488.74

Physical Properties

Property code	Value	Unit	Source
gf	-142.45	kJ/mol	Joback Method
hf	-944.99	kJ/mol	Joback Method
hfus	68.25	kJ/mol	Joback Method
hvap	103.89	kJ/mol	Joback Method
log10ws	-9.39		Crippen Method
logp	8.603		Crippen Method
mcvol	438.770	ml/mol	McGowan Method
pc	710.35	kPa	Joback Method
rinpol	3342.00		NIST Webbook
tb	1084.71	K	Joback Method
tc	1341.44	K	Joback Method
tf	612.29	K	Joback Method
vc	1.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1561.76	J/molxK	1084.71	Joback Method
cpg	1581.52	J/molxK	1127.50	Joback Method
cpg	1599.47	J/molxK	1170.29	Joback Method
cpg	1615.74	J/molxK	1213.08	Joback Method
cpg	1630.49	J/molxK	1255.86	Joback Method
cpg	1643.88	J/molxK	1298.65	Joback Method
cpg	1656.06	J/molxK	1341.44	Joback Method
dvisc	0.0001528	Paxs	612.29	Joback Method
dvisc	0.0000694	Paxs	691.03	Joback Method

dvisc	0.0000371	Paxs	769.76	Joback Method
dvisc	0.0000222	Paxs	848.50	Joback Method
dvisc	0.0000145	Paxs	927.24	Joback Method
dvisc	0.0000102	Paxs	1005.97	Joback Method
dvisc	0.0000075	Paxs	1084.71	Joback Method

Sources

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=U361628&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	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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