

Dimethylmalonic acid, 4-acetylphenyl heptadecyl ester

Inchi: InChI=1S/C30H48O5/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-24-34-28(32)30(3,4)2

InchiKey: AEJAZLHGFWHTFZ-UHFFFAOYSA-N

Formula: C30H48O5

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccc(C(C)=O)cc1

Mol. weight [g/mol]: 488.70

Physical Properties

Property code	Value	Unit	Source
gf	-289.42	kJ/mol	Joback Method
hf	-1048.40	kJ/mol	Joback Method
hfus	66.87	kJ/mol	Joback Method
hvap	109.07	kJ/mol	Joback Method
log10ws	-9.44		Crippen Method
logp	8.235		Crippen Method
mcvol	426.250	ml/mol	McGowan Method
pc	768.19	kPa	Joback Method
rinpol	3432.00		NIST Webbook
rinpol	3432.00		NIST Webbook
tb	1120.68	K	Joback Method
tc	1386.39	K	Joback Method
tf	663.47	K	Joback Method
vc	1.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1508.05	J/mol×K	1120.68	Joback Method
cpg	1525.03	J/mol×K	1164.97	Joback Method
cpg	1540.12	J/mol×K	1209.25	Joback Method
cpg	1553.46	J/mol×K	1253.54	Joback Method
cpg	1565.21	J/mol×K	1297.82	Joback Method
cpg	1575.51	J/mol×K	1342.11	Joback Method
cpg	1584.50	J/mol×K	1386.39	Joback Method
dvisc	0.0001201	Pa×s	663.47	Joback Method

dvisc	0.0000612	Pa×s	739.67	Joback Method
dvisc	0.0000354	Pa×s	815.87	Joback Method
dvisc	0.0000225	Pa×s	892.07	Joback Method
dvisc	0.0000153	Pa×s	968.28	Joback Method
dvisc	0.0000110	Pa×s	1044.48	Joback Method
dvisc	0.0000083	Pa×s	1120.68	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=U363710&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

Latest version available from:

<https://www.cheméo.com/cid/21-686-7/Dimethylmalonic-acid-4-acetylphenyl-heptadecyl-ester.pdf>

Generated by Cheméo on 2025-12-05 20:04:59.912425119 +0000 UTC m=+4713297.442465773.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.