

Malonic acid, 2,4-dimethylpent-3-yl heptadecyl ester

Inchi:	InChI=1S/C27H52O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-30-25(28)22-26(
InchiKey:	ZVMUTDVUFCEGMEU-UHFFFAOYSA-N
Formula:	C27H52O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	440.70

Physical Properties

Property code	Value	Unit	Source
gf	-298.70	kJ/mol	Joback Method
hf	-1106.05	kJ/mol	Joback Method
hfus	60.69	kJ/mol	Joback Method
hvap	92.84	kJ/mol	Joback Method
log10ws	-8.48		Crippen Method
logp	8.015		Crippen Method
mvol	406.170	ml/mol	McGowan Method
pc	732.84	kPa	Joback Method
rinpol	2861.00		NIST Webbook
tb	968.42	K	Joback Method
tc	1192.39	K	Joback Method
tf	493.37	K	Joback Method
vc	1.577	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1410.70	J/molxK	968.42	Joback Method
cpg	1500.22	J/molxK	1155.06	Joback Method
cpg	1485.71	J/molxK	1117.73	Joback Method
cpg	1469.56	J/molxK	1080.40	Joback Method
cpg	1451.72	J/molxK	1043.08	Joback Method
cpg	1432.11	J/molxK	1005.75	Joback Method
cpg	1513.15	J/molxK	1192.39	Joback Method
dvisc	0.0000140	Paxs	968.42	Joback Method
dvisc	0.0000196	Paxs	889.25	Joback Method

dvisc	0.0000295	Paxs	810.07	Joback Method
dvisc	0.0000484	Paxs	730.89	Joback Method
dvisc	0.0000895	Paxs	651.72	Joback Method
dvisc	0.0001964	Paxs	572.55	Joback Method
dvisc	0.0005544	Paxs	493.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349023&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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