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

Inchi: InChI=1S/C15H28O4/c1-6-7-8-9-18-13(16)10-14(17)19-15(11(2)3)12(4)5/h11-12,15H,6-1

InchiKey: FPIIEKZBRZSDAC-UHFFFAOYSA-N

Formula: C15H28O4

SMILES: CCCCCOC(=O)CC(=O)OC(C(C)C)C(C)C

Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
gf	-399.74	kJ/mol	Joback Method
hf	-858.37	kJ/mol	Joback Method
hfus	29.61	kJ/mol	Joback Method
hvap	66.13	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.334		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
rinpol	1677.00		NIST Webbook
tb	693.86	K	Joback Method
tc	876.51	K	Joback Method
tf	358.13	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.70	J/mol×K	693.86	Joback Method
cpg	695.52	J/mol×K	724.30	Joback Method
cpg	711.49	J/mol×K	754.74	Joback Method
cpg	726.61	J/mol×K	785.18	Joback Method
cpg	740.89	J/mol×K	815.62	Joback Method
cpg	754.34	J/mol×K	846.06	Joback Method
cpg	766.97	J/mol×K	876.51	Joback Method
dvisc	0.0027078	Pa×s	358.13	Joback Method
dvisc	0.0010257	Pa×s	414.08	Joback Method

dvisc	0.0004895	Pa×s	470.04	Joback Method
dvisc	0.0002735	Pa×s	526.00	Joback Method
dvisc	0.0001709	Pa×s	581.95	Joback Method
dvisc	0.0001159	Pa×s	637.90	Joback Method
dvisc	0.0000837	Pa×s	693.86	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=U349012&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.chemeo.com/cid/38-504-0/Malonic-acid-2-4-dimethylpent-3-yl-pentyl-ester.pdf
Generated by Cheméo on 2024-04-29 09:40:58.141229118 +0000 UTC m=+16672907.061806429.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.