Malonic acid, heptadecyl 4-methylpent-2-yl ester

Inchi: InChI=1S/C26H50O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-29-25(27)22-26(2

InchiKey: SYGIOFGABPXDRU-UHFFFAOYSA-N

Formula: C26H50O4

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

Mol. weight [g/mol]: 426.67

Physical Properties

Property code	Value	Unit	Source
gf	-304.68	kJ/mol	Joback Method
hf	-1080.13	kJ/mol	Joback Method
hfus	61.62	kJ/mol	Joback Method
hvap	91.01	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	7.769		Crippen Method
mcvol	392.080	ml/mol	McGowan Method
pc	769.04	kPa	Joback Method
rinpol	2772.00		NIST Webbook
rinpol	2772.00		NIST Webbook
tb	945.98	K	Joback Method
tc	1162.69	K	Joback Method
tf	497.10	K	Joback Method
vc	1.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.96	J/mol×K	945.98	Joback Method
cpg	1367.00	J/mol×K	982.10	Joback Method
cpg	1386.38	J/mol×K	1018.22	Joback Method
cpg	1404.14	J/mol×K	1054.33	Joback Method
cpg	1420.33	J/mol×K	1090.45	Joback Method
cpg	1435.00	J/mol×K	1126.57	Joback Method
cpg	1448.19	J/mol×K	1162.69	Joback Method
dvisc	0.0005428	Pa×s	497.10	Joback Method

dvisc	0.0002121	Pa×s	571.91	Joback Method
dvisc	0.0001030	Pa×s	646.73	Joback Method
dvisc	0.0000581	Pa×s	721.54	Joback Method
dvisc	0.0000365	Pa×s	796.35	Joback Method
dvisc	0.0000248	Pa×s	871.17	Joback Method
dvisc	0.0000180	Pa×s	945.98	Joback Method

Sources

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=U349344&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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