Malonic acid, 4-heptyl pentyl ester

Inchi: InChI=1S/C15H28O4/c1-4-7-8-11-18-14(16)12-15(17)19-13(9-5-2)10-6-3/h13H,4-12H2,1
InchiKey: SOBJQXWCJIIMNV-UHFFFAOYSA-N
Formula: C15H28O4
SMILES: CCCCCOC(=O)CC(=O)OC(CCC)CCC
Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
gf	-394.86	kJ/mol	Joback Method
hf	-847.81	kJ/mol	Joback Method
hfus	36.66	kJ/mol	Joback Method
hvap	66.91	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.622		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1528.27	kPa	Joback Method
rinpol	1718.00		NIST Webbook
tb	694.74	K	Joback Method
tc	872.74	K	Joback Method
tf	388.13	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.76	J/mol×K	694.74	Joback Method
cpg	694.10	J/mol×K	724.41	Joback Method
cpg	709.65	J/mol×K	754.07	Joback Method
cpg	724.41	J/mol×K	783.74	Joback Method
cpg	738.39	J/mol×K	813.41	Joback Method
cpg	751.59	J/mol×K	843.08	Joback Method
cpg	764.02	J/mol×K	872.74	Joback Method
dvisc	0.0016719	Pa×s	388.13	Joback Method
dvisc	0.0007909	Pa×s	439.23	Joback Method

dvisc	0.0004373	Pa×s	490.33	Joback Method
dvisc	0.0002704	Pa×s	541.43	Joback Method
dvisc	0.0001817	Pa×s	592.54	Joback Method
dvisc	0.0001300	Pa×s	643.64	Joback Method
dvisc	0.0000977	Pa×s	694.74	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=U348993&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

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