Malonic acid, 2-heptyl propyl ester

Inchi: InChI=1S/C13H24O4/c1-4-6-7-8-11(3)17-13(15)10-12(14)16-9-5-2/h11H,4-10H2,1-3H3
InchiKey: UNQUXNIACIMTOX-UHFFFAOYSA-N
Formula: C13H24O4
SMILES: CCCCCC(C)OC(=O)CC(=O)OCCC
Mol. weight [g/mol]: 244.33

Physical Properties

Property code	Value	Unit	Source
gf	-411.70	kJ/mol	Joback Method
hf	-806.53	kJ/mol	Joback Method
hfus	31.48	kJ/mol	Joback Method
hvap	62.46	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.842		Crippen Method
mcvol	208.910	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	1554.00		NIST Webbook
rinpol	1554.00		NIST Webbook
tb	648.98	K	Joback Method
tc	828.08	K	Joback Method
tf	365.59	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.82	J/mol×K	648.98	Joback Method
cpg	584.20	J/mol×K	678.83	Joback Method
cpg	598.88	J/mol×K	708.68	Joback Method
cpg	612.86	J/mol×K	738.53	Joback Method
cpg	626.13	J/mol×K	768.38	Joback Method
cpg	638.71	J/mol×K	798.23	Joback Method
cpg	650.59	J/mol×K	828.08	Joback Method
dvisc	0.0019834	Pa×s	365.59	Joback Method

dvisc	0.0009630	Pa×s	412.82	Joback Method
dvisc	0.0005423	Pa×s	460.05	Joback Method
dvisc	0.0003399	Pa×s	507.29	Joback Method
dvisc	0.0002306	Pa×s	554.52	Joback Method
dvisc	0.0001663	Pa×s	601.75	Joback Method
dvisc	0.0001258	Pa×s	648.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349130&Units=SI
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

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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