

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:	CCCCC(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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0009630	Paxs	412.82	Joback Method
dvisc	0.0005423	Paxs	460.05	Joback Method
dvisc	0.0003399	Paxs	507.29	Joback Method
dvisc	0.0002306	Paxs	554.52	Joback Method
dvisc	0.0001663	Paxs	601.75	Joback Method
dvisc	0.0001258	Paxs	648.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349130&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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