

Malonic acid, 2-heptyl hexyl ester

Inchi:	InChI=1S/C16H30O4/c1-4-6-8-10-12-19-15(17)13-16(18)20-14(3)11-9-7-5-2/h14H,4-13H
InchiKey:	FROFWPXQIKSQFR-UHFFFAOYSA-N
Formula:	C16H30O4
SMILES:	CCCCCOC(=O)CC(=O)OC(C)CCCC
Mol. weight [g/mol]:	286.41

Physical Properties

Property code	Value	Unit	Source
gf	-386.44	kJ/mol	Joback Method
hf	-868.45	kJ/mol	Joback Method
hfus	39.25	kJ/mol	Joback Method
hvap	69.13	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.012		Crippen Method
mvol	251.180	ml/mol	McGowan Method
pc	1419.71	kPa	Joback Method
rinpol	1841.00		NIST Webbook
rinpol	1841.00		NIST Webbook
tb	717.62	K	Joback Method
tc	895.76	K	Joback Method
tf	399.40	K	Joback Method
vc	0.974	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.08	J/molxK	717.62	Joback Method
cpg	750.85	J/molxK	747.31	Joback Method
cpg	766.77	J/molxK	777.00	Joback Method
cpg	781.86	J/molxK	806.69	Joback Method
cpg	796.13	J/molxK	836.38	Joback Method
cpg	809.59	J/molxK	866.07	Joback Method
cpg	822.23	J/molxK	895.76	Joback Method
dvisc	0.0015210	Paxs	399.40	Joback Method

dvisc	0.0007109	Paxs	452.44	Joback Method
dvisc	0.0003898	Paxs	505.47	Joback Method
dvisc	0.0002395	Paxs	558.51	Joback Method
dvisc	0.0001602	Paxs	611.55	Joback Method
dvisc	0.0001142	Paxs	664.58	Joback Method
dvisc	0.0000856	Paxs	717.62	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=U349135&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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