

Malonic acid, 3-heptyl isohexyl ester

Inchi:	InChI=1S/C16H30O4/c1-5-7-10-14(6-2)20-16(18)12-15(17)19-11-8-9-13(3)4/h13-14H,5-
InchiKey:	NOKXZCOJQOZQQT-UHFFFAOYSA-N
Formula:	C16H30O4
SMILES:	CCCCC(CC)OC(=O)CC(=O)OCCCC(C)C
Mol. weight [g/mol]:	286.41

Physical Properties

Property code	Value	Unit	Source
gf	-388.88	kJ/mol	Joback Method
hf	-873.73	kJ/mol	Joback Method
hfus	35.72	kJ/mol	Joback Method
hvap	68.75	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.868		Crippen Method
mvol	251.180	ml/mol	McGowan Method
pc	1428.30	kPa	Joback Method
rinpol	1777.00		NIST Webbook
rinpol	1777.00		NIST Webbook
tb	717.18	K	Joback Method
tc	897.32	K	Joback Method
tf	384.40	K	Joback Method
vc	0.968	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.56	J/molxK	717.18	Joback Method
cpg	751.53	J/molxK	747.20	Joback Method
cpg	767.64	J/molxK	777.23	Joback Method
cpg	782.89	J/molxK	807.25	Joback Method
cpg	797.29	J/molxK	837.27	Joback Method
cpg	810.84	J/molxK	867.29	Joback Method
cpg	823.57	J/molxK	897.32	Joback Method
dvisc	0.0018907	Paxs	384.40	Joback Method

dvisc	0.0007981	Paxs	439.86	Joback Method
dvisc	0.0004087	Paxs	495.33	Joback Method
dvisc	0.0002395	Paxs	550.79	Joback Method
dvisc	0.0001547	Paxs	606.25	Joback Method
dvisc	0.0001076	Paxs	661.72	Joback Method
dvisc	0.0000791	Paxs	717.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349151&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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