

Malonic acid, 10-chlorodecyl isobutyl ester

Inchi:	InChI=1S/C17H31ClO4/c1-15(2)14-22-17(20)13-16(19)21-12-10-8-6-4-3-5-7-9-11-18/h15
InchiKey:	IJONSIOAQZMZJJ-UHFFFAOYSA-N
Formula:	C17H31ClO4
SMILES:	CC(C)COC(=O)CC(=O)OCCCCCCCCCCI
Mol. weight [g/mol]:	334.88

Physical Properties

Property code	Value	Unit	Source
gf	-389.95	kJ/mol	Joback Method
hf	-904.83	kJ/mol	Joback Method
hfus	46.03	kJ/mol	Joback Method
hvap	75.75	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.478		Crippen Method
mvol	277.510	ml/mol	McGowan Method
pc	1287.44	kPa	Joback Method
rinpol	2281.00		NIST Webbook
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tb	777.93	K	Joback Method
tc	962.16	K	Joback Method
tf	440.59	K	Joback Method
vc	1.079	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.99	J/molxK	777.93	Joback Method
cpg	895.16	J/molxK	931.45	Joback Method
cpg	882.53	J/molxK	900.75	Joback Method
cpg	869.00	J/molxK	870.04	Joback Method
cpg	854.58	J/molxK	839.34	Joback Method
cpg	839.25	J/molxK	808.63	Joback Method
cpg	906.92	J/molxK	962.16	Joback Method
dvisc	0.0000650	Paxs	777.93	Joback Method

dvisc	0.0000866	Paxs	721.71	Joback Method
dvisc	0.0001209	Paxs	665.48	Joback Method
dvisc	0.0001797	Paxs	609.26	Joback Method
dvisc	0.0002895	Paxs	553.04	Joback Method
dvisc	0.0005194	Paxs	496.81	Joback Method
dvisc	0.0010819	Paxs	440.59	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349040&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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