

Malonic acid, di(8-chlorooctyl) ester

Inchi:	InChI=1S/C19H34Cl2O4/c20-13-9-5-1-3-7-11-15-24-18(22)17-19(23)25-16-12-8-4-2-6-10
InchiKey:	XPFJQQXPWSKDES-UHFFFAOYSA-N
Formula:	C19H34Cl2O4
SMILES:	O=C(CC(=O)OCCCCCCCCCl)OCCCCCCCCCl
Mol. weight [g/mol]:	397.38

Physical Properties

Property code	Value	Unit	Source
gf	-382.60	kJ/mol	Joback Method
hf	-956.57	kJ/mol	Joback Method
hfus	58.93	kJ/mol	Joback Method
hvap	84.97	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.622		Crippen Method
mvol	317.930	ml/mol	McGowan Method
pc	1093.54	kPa	Joback Method
rinpol	2843.00		NIST Webbook
rinpol	2843.00		NIST Webbook
tb	861.56	K	Joback Method
tc	1056.00	K	Joback Method
tf	508.05	K	Joback Method
vc	1.246	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.07	J/mol×K	861.56	Joback Method
cpg	1039.68	J/mol×K	1023.59	Joback Method
cpg	1027.81	J/mol×K	991.19	Joback Method
cpg	1014.94	J/mol×K	958.78	Joback Method
cpg	1001.04	J/mol×K	926.37	Joback Method
cpg	986.09	J/mol×K	893.97	Joback Method
cpg	1050.57	J/mol×K	1056.00	Joback Method
dvisc	0.0000449	Paxs	861.56	Joback Method

dvisc	0.0000589	Paxs	802.64	Joback Method
dvisc	0.0000806	Paxs	743.72	Joback Method
dvisc	0.0001164	Paxs	684.80	Joback Method
dvisc	0.0001802	Paxs	625.89	Joback Method
dvisc	0.0003055	Paxs	566.97	Joback Method
dvisc	0.0005853	Paxs	508.05	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=U349007&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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