

Myristic acid, 3,4-dichlorophenyl ester

Inchi:	InChI=1S/C20H30Cl2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-20(23)24-17-14-15-18(21)19(22)
InchiKey:	UGDWGXYFBAYMQX-UHFFFAOYSA-N
Formula:	C20H30Cl2O2
SMILES:	CCCCCCCCCCCC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	373.36

Physical Properties

Property code	Value	Unit	Source
gf	-47.11	kJ/mol	Joback Method
hf	-518.82	kJ/mol	Joback Method
hfus	52.00	kJ/mol	Joback Method
hvap	81.64	kJ/mol	Joback Method
log10ws	-8.18		Crippen Method
logp	7.600		Crippen Method
mvol	300.820	ml/mol	McGowan Method
pc	1218.29	kPa	Joback Method
rinpol	2688.00		NIST Webbook
tb	844.79	K	Joback Method
tc	1046.64	K	Joback Method
tf	498.62	K	Joback Method
vc	1.169	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.46	J/molxK	844.79	Joback Method
cpg	901.40	J/molxK	878.43	Joback Method
cpg	916.31	J/molxK	912.07	Joback Method
cpg	930.20	J/molxK	945.72	Joback Method
cpg	943.13	J/molxK	979.36	Joback Method
cpg	955.13	J/molxK	1013.00	Joback Method
cpg	966.23	J/molxK	1046.64	Joback Method
dvisc	0.0005909	Paxs	498.62	Joback Method
dvisc	0.0003276	Paxs	556.32	Joback Method

dvisc	0.0002030	Paxs	614.01	Joback Method
dvisc	0.0001365	Paxs	671.70	Joback Method
dvisc	0.0000978	Paxs	729.40	Joback Method
dvisc	0.0000735	Paxs	787.10	Joback Method
dvisc	0.0000575	Paxs	844.79	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357931&Units=SI

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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