

Octadecyl formate

Inchi:	InChI=1S/C19H38O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-19-20/h19H,2-
InchiKey:	NOPZJEGEHWZSE-UHFFFAOYSA-N
Formula:	C19H38O2
SMILES:	CCCCCCCCCCCCCCCCCOC=O
Mol. weight [g/mol]:	298.50
CAS:	5451-75-2

Physical Properties

Property code	Value	Unit	Source
gf	-95.42	kJ/mol	Joback Method
hf	-653.29	kJ/mol	Joback Method
hfus	48.44	kJ/mol	Joback Method
hvap	67.02	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	6.421		Crippen Method
mvol	286.010	ml/mol	McGowan Method
pc	1122.31	kPa	Joback Method
rinpol	2118.00		NIST Webbook
rinpol	2118.00		NIST Webbook
tb	705.20	K	Joback Method
tc	872.48	K	Joback Method
tf	368.12	K	Joback Method
vc	1.135	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.46	J/molxK	705.20	Joback Method
cpg	866.49	J/molxK	733.08	Joback Method
cpg	884.68	J/molxK	760.96	Joback Method
cpg	902.04	J/molxK	788.84	Joback Method
cpg	918.59	J/molxK	816.72	Joback Method
cpg	934.36	J/molxK	844.60	Joback Method
cpg	949.37	J/molxK	872.48	Joback Method

dvisc	0.0021420	Paxs	368.12	Joback Method
dvisc	0.0008989	Paxs	424.30	Joback Method
dvisc	0.0004621	Paxs	480.48	Joback Method
dvisc	0.0002731	Paxs	536.66	Joback Method
dvisc	0.0001783	Paxs	592.84	Joback Method
dvisc	0.0001253	Paxs	649.02	Joback Method
dvisc	0.0000932	Paxs	705.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.64610e+01
Coeff. B	-1.04734e+04
Coeff. C	-1.33568e+02
Temperature range (K), min.	533.72
Temperature range (K), max.	628.77

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=R543538&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rincpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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