

13-docosenoic acid

Inchi:	InChI=1S/C22H42O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(23)24
InchiKey:	DPUOLQHDNGRHBS-UHFFFAOYSA-N
Formula:	C22H42O2
SMILES:	CCCCCCCC=CCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	338.57
CAS:	1072-39-5

Physical Properties

Property code	Value	Unit	Source
gf	-51.16	kJ/mol	Joback Method
hf	-645.00	kJ/mol	Joback Method
hfus	58.62	kJ/mol	Joback Method
hvap	87.95	kJ/mol	Joback Method
log10ws	-7.98		Crippen Method
logp	7.669		Crippen Method
mcvol	323.980	ml/mol	McGowan Method
pc	1025.31	kPa	Joback Method
tb	852.97	K	Joback Method
tc	1044.39	K	Joback Method
tf	334.65 ± 1.00	K	NIST Webbook
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1052.00	J/molxK	852.97	Joback Method
cpg	1070.89	J/molxK	884.87	Joback Method
cpg	1088.82	J/molxK	916.78	Joback Method
cpg	1105.83	J/molxK	948.68	Joback Method
cpg	1121.99	J/molxK	980.59	Joback Method
cpg	1137.36	J/molxK	1012.49	Joback Method
cpg	1152.00	J/molxK	1044.39	Joback Method
dvisc	0.0010953	Paxs	443.37	Joback Method
dvisc	0.0002981	Paxs	511.64	Joback Method

dvisc	0.0001102	Paxs	579.90	Joback Method
dvisc	0.0000503	Paxs	648.17	Joback Method
dvisc	0.0000266	Paxs	716.44	Joback Method
dvisc	0.0000157	Paxs	784.70	Joback Method
dvisc	0.0000101	Paxs	852.97	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.66104e+01
Coeff. B	-6.84544e+03
Coeff. C	-1.42742e+02
Temperature range (K), min.	562.12
Temperature range (K), max.	748.59

Sources

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
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=C1072395&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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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