

2-Ethyleicosanoic acid

Inchi:	InChI=1S/C22H44O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(4-2)22(23)24
InchiKey:	MBFSRSJRTRVYJN-UHFFFAOYSA-N
Formula:	C22H44O2
SMILES:	CCCCCCCCCCCCCCCCCCC(CC)C(=O)O
Mol. weight [g/mol]:	340.58

Physical Properties

Property code	Value	Unit	Source
gf	-133.82	kJ/mol	Joback Method
hf	-767.50	kJ/mol	Joback Method
hfus	54.90	kJ/mol	Joback Method
hvap	87.60	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	7.749		Crippen Method
mcvol	328.280	ml/mol	McGowan Method
pc	997.02	kPa	Joback Method
rinpol	2377.00		NIST Webbook
rinpol	2377.00		NIST Webbook
tb	848.37	K	Joback Method
tc	1038.91	K	Joback Method
tf	433.45	K	Joback Method
vc	1.286	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1078.51	J/molxK	848.37	Joback Method
cpg	1098.03	J/molxK	880.13	Joback Method
cpg	1116.49	J/molxK	911.88	Joback Method
cpg	1133.93	J/molxK	943.64	Joback Method
cpg	1150.42	J/molxK	975.39	Joback Method
cpg	1165.99	J/molxK	1007.15	Joback Method
cpg	1180.69	J/molxK	1038.91	Joback Method
dvisc	0.0015132	Paxs	433.45	Joback Method

dvisc	0.0003761	Paxs	502.60	Joback Method
dvisc	0.0001309	Paxs	571.76	Joback Method
dvisc	0.0000572	Paxs	640.91	Joback Method
dvisc	0.0000294	Paxs	710.06	Joback Method
dvisc	0.0000170	Paxs	779.22	Joback Method
dvisc	0.0000107	Paxs	848.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R435591&Units=SI
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

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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