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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1078.51	J/mol×K	848.37	Joback Method
cpg	1165.99	J/mol×K	1007.15	Joback Method
cpg	1150.42	J/mol×K	975.39	Joback Method
cpg	1133.93	J/mol×K	943.64	Joback Method
cpg	1116.49	J/mol×K	911.88	Joback Method
cpg	1098.03	J/mol×K	880.13	Joback Method
cpg	1180.69	J/mol×K	1038.91	Joback Method
dvisc	0.0000107	Pa×s	848.37	Joback Method

dvisc	0.0000170	Pa×s	779.22	Joback Method
dvisc	0.0000294	Pa×s	710.06	Joback Method
dvisc	0.0000572	Pa×s	640.91	Joback Method
dvisc	0.0001309	Pa×s	571.76	Joback Method
dvisc	0.0003761	Pa×s	502.60	Joback Method
dvisc	0.0015132	Pa×s	433.45	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=R435591&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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