Eicosanedioic acid

Inchi: InChI=1S/C20H38O4/c21-19(22)17-15-13-11-9-7-5-3-1-2-4-6-8-10-12-14-16-18-20(23)24
InchiKey: JJOJFIHJIRWASH-UHFFFAOYSA-N
Formula: C20H38O4
SMILES: O=C(O)CCCCCCCCCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]: 342.51
CAS: 2424-92-2

Physical Properties

Property code	Value	Unit	Source
gf	-413.96	kJ/mol	Joback Method
hf	-985.75	kJ/mol	Joback Method
hfus	58.93	kJ/mol	Joback Method
hsub	170.00 ± 3.30	kJ/mol	NIST Webbook
hsub	166.00 ± 3.00	kJ/mol	NIST Webbook
hvap	106.96	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	6.177		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1250.38	kPa	Joback Method
tb	949.10	K	Joback Method
tc	1171.59	K	Joback Method
tf	536.66	K	Joback Method
vc	1.206	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1117.04	J/mol×K	1134.50	Joback Method
cpg	1128.85	J/mol×K	1171.59	Joback Method
cpg	1043.79	J/mol×K	949.10	Joback Method
cpg	1060.57	J/mol×K	986.18	Joback Method
cpg	1076.21	J/mol×K	1023.26	Joback Method
cpg	1090.79	J/mol×K	1060.34	Joback Method
cpg	1104.38	J/mol×K	1097.42	Joback Method

dvisc	0.0000017	Pa×s	949.10	Joback Method
dvisc	0.0000027	Pa×s	880.36	Joback Method
dvisc	0.0002368	Pa×s	536.66	Joback Method
dvisc	0.0000648	Pa×s	605.40	Joback Method
dvisc	0.0000231	Pa×s	674.14	Joback Method
dvisc	0.0000100	Pa×s	742.88	Joback Method
dvisc	0.0000050	Pa×s	811.62	Joback Method
hsubt	165.70 ± 3.30	kJ/mol	387.50	NIST Webbook
hsubt	199.50	kJ/mol	341.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	506.70	K	0.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2424922&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume