

cis-13,16-Docasadienoic acid

Inchi:	InChI=1S/C22H40O2/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:	HVGRZDASOHMCSK-HZJYTTRNSA-N
Formula:	C22H40O2
SMILES:	CCCCC=CCC=CCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	336.55
CAS:	7370-49-2

Physical Properties

Property code	Value	Unit	Source
gf	29.06	kJ/mol	Joback Method
hf	-527.78	kJ/mol	Joback Method
hfus	58.83	kJ/mol	Joback Method
hvap	87.91	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	7.445		Crippen Method
mcvol	319.680	ml/mol	McGowan Method
pc	1060.33	kPa	Joback Method
rinpol	2566.20		NIST Webbook
rinpol	2566.20		NIST Webbook
tb	857.13	K	Joback Method
tc	1049.37	K	Joback Method
tf	438.29	K	Joback Method
vc	1.252	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1025.76	J/mol×K	857.13	Joback Method
cpg	1108.97	J/mol×K	1017.33	Joback Method
cpg	1093.82	J/mol×K	985.29	Joback Method
cpg	1077.99	J/mol×K	953.25	Joback Method
cpg	1061.42	J/mol×K	921.21	Joback Method
cpg	1044.03	J/mol×K	889.17	Joback Method
cpg	1123.52	J/mol×K	1049.37	Joback Method

dvisc	0.0000088	Paxs	857.13	Joback Method
dvisc	0.0000137	Paxs	787.32	Joback Method
dvisc	0.0000233	Paxs	717.52	Joback Method
dvisc	0.0000444	Paxs	647.71	Joback Method
dvisc	0.0000990	Paxs	577.90	Joback Method
dvisc	0.0002752	Paxs	508.10	Joback Method
dvisc	0.0010596	Paxs	438.29	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7370492&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
mvol:	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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