

Tricosanal

Inchi: InChI=1S/C23H46O/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: IALIDHPAWNTXOK-UHFFFAOYSA-N
Formula: C23H46O
SMILES: CCCCCCCCCCCCCCCCCCCCCC=O
Mol. weight [g/mol]: 338.61
CAS: 72934-02-2

Physical Properties

Property code	Value	Unit	Source
gf	43.26	kJ/mol	Joback Method
hf	-603.63	kJ/mol	Joback Method
hfus	57.62	kJ/mol	Joback Method
hvap	73.51	kJ/mol	Joback Method
log10ws	-8.73		Crippen Method
logp	8.397		Crippen Method
mcvol	336.500	ml/mol	McGowan Method
pc	890.00	kPa	Joback Method
rinpol	2534.40		NIST Webbook
rinpol	2511.00		NIST Webbook
rinpol	2531.00		NIST Webbook
tb	774.30	K	Joback Method
tc	949.27	K	Joback Method
tf	390.97	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.64	J/molxK	774.30	Joback Method
cpg	1078.76	J/molxK	803.46	Joback Method
cpg	1098.87	J/molxK	832.62	Joback Method
cpg	1118.00	J/molxK	861.79	Joback Method
cpg	1136.21	J/molxK	890.95	Joback Method
cpg	1153.52	J/molxK	920.11	Joback Method

cpg	1169.98	J/molxK	949.27	Joback Method
dvisc	0.0021077	Paxs	390.97	Joback Method
dvisc	0.0008080	Paxs	454.86	Joback Method
dvisc	0.0003923	Paxs	518.75	Joback Method
dvisc	0.0002232	Paxs	582.63	Joback Method
dvisc	0.0001419	Paxs	646.52	Joback Method
dvisc	0.0000979	Paxs	710.41	Joback Method
dvisc	0.0000718	Paxs	774.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72934022&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

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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