

Ethyl henicosanoate

Inchi:	InChI=1S/C23H46O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(24)25
InchiKey:	BKTDTEKUOZFAMW-UHFFFAOYSA-N
Formula:	C23H46O2
SMILES:	CCCCCCCCCCCCCCCCCCCC(=O)OCC
Mol. weight [g/mol]:	354.61
CAS:	28898-67-1

Physical Properties

Property code	Value	Unit	Source
gf	-91.14	kJ/mol	Joback Method
hf	-762.85	kJ/mol	Joback Method
hfus	58.11	kJ/mol	Joback Method
hvap	75.95	kJ/mol	Joback Method
log10ws	-8.31		Crippen Method
logp	7.981		Crippen Method
mcvol	342.370	ml/mol	McGowan Method
pc	875.32	kPa	Joback Method
rinpol	2492.10		NIST Webbook
rinpol	2492.10		NIST Webbook
tb	801.93	K	Joback Method
tc	982.34	K	Joback Method
tf	421.13	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.53	J/molxK	801.93	Joback Method
cpg	1114.64	J/molxK	832.00	Joback Method
cpg	1134.65	J/molxK	862.07	Joback Method
cpg	1153.61	J/molxK	892.14	Joback Method
cpg	1171.55	J/molxK	922.21	Joback Method
cpg	1188.50	J/molxK	952.27	Joback Method
cpg	1204.49	J/molxK	982.34	Joback Method

dvisc	0.0011936	Paxs	421.13	Joback Method
dvisc	0.0004928	Paxs	484.60	Joback Method
dvisc	0.0002498	Paxs	548.06	Joback Method
dvisc	0.0001457	Paxs	611.53	Joback Method
dvisc	0.0000941	Paxs	675.00	Joback Method
dvisc	0.0000655	Paxs	738.46	Joback Method
dvisc	0.0000483	Paxs	801.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28898671&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
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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