3-Tetradecyn-1-ol

Inchi: InChI=1S/C14H26O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15/h15H,2-10,13-14H2,1H3
InchiKey: MDMMHGIVSNOJID-UHFFFAOYSA-N
Formula: C14H26O
SMILES: CCCCCCCCCCC#CCCO
Mol. weight [g/mol]: 210.36
CAS: 55182-74-6

Physical Properties

Property code	Value	Unit	Source
gf	132.98	kJ/mol	Joback Method
hf	-212.22	kJ/mol	Joback Method
hfus	39.23	kJ/mol	Joback Method
hvap	65.59	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.903		Crippen Method
mcvol	205.390	ml/mol	McGowan Method
pc	1874.03	kPa	Joback Method
tb	620.90	K	Joback Method
tc	792.43	K	Joback Method
tf	414.46	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.16	J/mol×K	620.90	Joback Method
cpg	558.42	J/mol×K	649.49	Joback Method
cpg	573.03	J/mol×K	678.08	Joback Method
cpg	587.02	J/mol×K	706.67	Joback Method
cpg	600.40	J/mol×K	735.26	Joback Method
cpg	613.19	J/mol×K	763.84	Joback Method
cpg	625.42	J/mol×K	792.43	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63138e+01
Coeff. B	-5.69606e+03
Coeff. C	-1.06018e+02
Temperature range (K), min.	461.15
Temperature range (K), max.	624.15

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=C55182746&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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