4-Tridecanol

Other names: tridecan-4-ol
Inchi: InChI=1S/C13H28O/c1-3-5-6-7-8-9-10-12-13(14)11-4-2/h13-14H,3-12H2,1-2H3
InchiKey: VHNLHPIEIIHMHH-UHFFFAOYSA-N
Formula: C13H28O
SMILES: CCCCCCCCCC(O)CCC
Mol. weight [g/mol]: 200.36
CAS: 26215-92-9

Physical Properties

Property code	Value	Unit	Source
gf	-80.68	kJ/mol	Joback Method
hf	-469.16	kJ/mol	Joback Method
hfus	29.99	kJ/mol	Joback Method
hvap	60.82	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.288		Crippen Method
mcvol	199.900	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	1582.00		NIST Webbook
rinpol	1582.00		NIST Webbook
ripol	1856.00		NIST Webbook
ripol	1887.00		NIST Webbook
ripol	1887.00		NIST Webbook
ripol	1862.00		NIST Webbook
ripol	1856.00		NIST Webbook
tb	588.58	K	Joback Method
tc	748.59	K	Joback Method
tf	282.09	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.09	J/mol×K	588.58	Joback Method

cpg	545.60	J/mol×K	615.25	Joback Method
cpg	560.50	J/mol×K	641.92	Joback Method
cpg	574.79	J/mol×K	668.59	Joback Method
cpg	588.50	J/mol×K	695.25	Joback Method
cpg	601.64	J/mol×K	721.92	Joback Method
cpg	614.23	J/mol×K	748.59	Joback Method
dvisc	0.0293029	Pa×s	282.09	Joback Method
dvisc	0.0048963	Pa×s	333.17	Joback Method
dvisc	0.0013165	Pa×s	384.25	Joback Method
dvisc	0.0004818	Pa×s	435.33	Joback Method
dvisc	0.0002178	Pa×s	486.42	Joback Method
dvisc	0.0001145	Pa×s	537.50	Joback Method
dvisc	0.0000673	Pa×s	588.58	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56774e+01
Coeff. B	-4.99511e+03
Coeff. C	-8.95880e+01
Temperature range (K), min.	414.16
Temperature range (K), max.	571.46

Sources

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=C26215929&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

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume