

11-Tridecyn-1-ol

Inchi:	InChI=1S/C13H24O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14/h14H,4-13H2,1H3
InchiKey:	QBYUWRZJJAYBJR-UHFFFAOYSA-N
Formula:	C13H24O
SMILES:	CC#CCCCCCCCCCCO
Mol. weight [g/mol]:	196.33
CAS:	33925-75-6

Physical Properties

Property code	Value	Unit	Source
gf	124.56	kJ/mol	Joback Method
hf	-191.58	kJ/mol	Joback Method
hfus	36.64	kJ/mol	Joback Method
hvap	63.36	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.513		Crippen Method
mcvol	191.300	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
tb	598.02	K	Joback Method
tc	770.36	K	Joback Method
tf	403.19	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.48	J/mol×K	598.02	Joback Method
cpg	506.14	J/mol×K	626.74	Joback Method
cpg	520.19	J/mol×K	655.47	Joback Method
cpg	533.64	J/mol×K	684.19	Joback Method
cpg	546.51	J/mol×K	712.91	Joback Method
cpg	558.82	J/mol×K	741.64	Joback Method
cpg	570.60	J/mol×K	770.36	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.63240e+01
Coeff. B	-5.56023e+03
Coeff. C	-1.01387e+02
Temperature range (K), min.	448.15
Temperature range (K), max.	606.15

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=C33925756&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
mccvol:	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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