

3-Decyn-1-ol

Inchi:	InChI=1S/C10H18O/c1-2-3-4-5-6-7-8-9-10-11/h11H,2-6,9-10H2,1H3
InchiKey:	YGEQBZUDPQQIFI-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	CCCCCCC#CCCO
Mol. weight [g/mol]:	154.25
CAS:	51721-39-2

Physical Properties

Property code	Value	Unit	Source
gf	99.30	kJ/mol	Joback Method
hf	-129.66	kJ/mol	Joback Method
hfus	28.87	kJ/mol	Joback Method
hvap	56.69	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.343		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
tb	529.38	K	Joback Method
tc	705.61	K	Joback Method
tf	369.38	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.13	J/mol×K	529.38	Joback Method
cpg	358.61	J/mol×K	558.75	Joback Method
cpg	370.58	J/mol×K	588.12	Joback Method
cpg	382.05	J/mol×K	617.50	Joback Method
cpg	393.04	J/mol×K	646.87	Joback Method
cpg	403.56	J/mol×K	676.24	Joback Method
cpg	413.63	J/mol×K	705.61	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	403.50 ± 0.50	K	2.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.63622e+01
Coeff. B	-5.10696e+03
Coeff. C	-8.59310e+01
Temperature range (K), min.	403.15
Temperature range (K), max.	548.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51721392&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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