9-Dodecyn-1-ol

Inchi: InChI=1S/C12H22O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h13H,2,5-12H2,1H3
InchiKey: MIDXCKJJIFQOLT-UHFFFAOYSA-N
Formula: C12H22O
SMILES: CCC#CCCCCCCCCO
Mol. weight [g/mol]: 182.30
CAS: 71084-08-7

Physical Properties

Property code	Value	Unit	Source
gf	116.14	kJ/mol	Joback Method
hf	-170.94	kJ/mol	Joback Method
hfus	34.05	kJ/mol	Joback Method
hvap	61.14	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.123		Crippen Method
mcvol	177.210	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	1543.00		NIST Webbook
rinpol	1543.00		NIST Webbook
tb	575.14	K	Joback Method
tc	748.57	K	Joback Method
tf	391.92	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.34	J/mol×K	575.14	Joback Method
cpg	455.35	J/mol×K	604.05	Joback Method
cpg	468.78	J/mol×K	632.95	Joback Method
cpg	481.64	J/mol×K	661.86	Joback Method
cpg	493.95	J/mol×K	690.76	Joback Method
cpg	505.73	J/mol×K	719.67	Joback Method
cpg	517.00	J/mol×K	748.57	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63353e+01
Coeff. B	-5.41743e+03
Coeff. C	-9.65180e+01
Temperature range (K), min.	434.15
Temperature range (K), max.	588.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71084087&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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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