4-Dodecyne

Inchi: InChI=1S/C12H22/c1-3-5-7-9-11-12-10-8-6-4-2/h3-7,9,11-12H2,1-2H3
InchiKey: RVIMTVIYJAEION-UHFFFAOYSA-N
Formula: C12H22
SMILES: CCCC#CCCCCCCC
Mol. weight [g/mol]: 166.30
CAS: 22058-01-1

Physical Properties

Property code	Value	Unit	Source
gf	252.96	kJ/mol	Joback Method
hf	-18.71	kJ/mol	Joback Method
hfus	29.96	kJ/mol	Joback Method
hvap	44.46	kJ/mol	Joback Method
ie	9.14 ± 0.03	eV	NIST Webbook
log10ws	-4.64		Crippen Method
logp	4.150		Crippen Method
mcvol	171.340	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
rinpol	1203.00		NIST Webbook
rinpol	1202.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1203.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1203.00		NIST Webbook
rinpol	1203.00		NIST Webbook
rinpol	1209.00		NIST Webbook
rinpol	1229.00		NIST Webbook
ripol	1381.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1381.00		NIST Webbook
ripol	1388.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1388.00		NIST Webbook
ripol	1388.00		NIST Webbook

ripol	1388.00		NIST Webbook
ripol	1359.70		NIST Webbook
ripol	1362.70		NIST Webbook
ripol	1379.50		NIST Webbook
ripol	1365.30		NIST Webbook
tb	482.96	K	Joback Method
tc	664.00	K	Joback Method
tf	331.10	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.85	J/mol×K	482.96	Joback Method
cpg	393.20	J/mol×K	513.13	Joback Method
cpg	408.87	J/mol×K	543.31	Joback Method
cpg	423.89	J/mol×K	573.48	Joback Method
cpg	438.29	J/mol×K	603.66	Joback Method
cpg	452.07	J/mol×K	633.83	Joback Method
cpg	465.26	J/mol×K	664.00	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.31568e+01
Coeff. B	-2.99546e+03
Coeff. C	-1.36886e+02
Temperature range (K), min.	369.65
Temperature range (K), max.	518.70

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=C22058011&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
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
ie:	Ionization energy
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