6-Tridecyne

Other names: 6-C13H24
6-Tridecane
Inchi: InChI=1S/C13H24/c1-3-5-7-9-11-13-12-10-8-6-4-2/h3-11H2,1-2H3
InchiKey: DFZSEVCTTZHGAS-UHFFFAOYSA-N
Formula: C13H24
SMILES: CCCCCC#CCCCCCC
Mol. weight [g/mol]: 180.33
CAS: 42371-66-4

Physical Properties

Property code	Value	Unit	Source
gf	261.38	kJ/mol	Joback Method
hf	-39.35	kJ/mol	Joback Method
hfus	32.55	kJ/mol	Joback Method
hvap	46.68	kJ/mol	Joback Method
ie	9.05 ± 0.03	eV	NIST Webbook
log10ws	-5.06		Crippen Method
logp	4.540		Crippen Method
mcvol	185.430	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	1320.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1296.00		NIST Webbook
ripol	1449.10		NIST Webbook
ripol	1479.00		NIST Webbook
ripol	1479.00		NIST Webbook
ripol	1480.00		NIST Webbook
ripol	1477.00		NIST Webbook
ripol	1466.50		NIST Webbook
ripol	1452.60		NIST Webbook
ripol	1469.40		NIST Webbook
ripol	1477.00		NIST Webbook
ripol	1449.10		NIST Webbook
ripol	1478.00		NIST Webbook
tb	505.84	K	Joback Method

tc	685.15	K	Joback Method
tf	342.37	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.07	J/mol×K	505.84	Joback Method
cpg	441.19	J/mol×K	535.72	Joback Method
cpg	457.61	J/mol×K	565.61	Joback Method
cpg	473.34	J/mol×K	595.49	Joback Method
cpg	488.41	J/mol×K	625.38	Joback Method
cpg	502.83	J/mol×K	655.26	Joback Method
cpg	516.62	J/mol×K	685.15	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.77276e+01
Coeff. B	-6.88343e+03
Coeff. C	1.87420e+01
Temperature range (K), min.	375.95
Temperature range (K), max.	535.65

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=C42371664&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
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