12-Ethyltricosane

Inchi: InChI=1S/C25H52/c1-4-7-9-11-13-15-17-19-21-23-25(6-3)24-22-20-18-16-14-12-10-8-5-2

InchiKey: IDYSNLVYORVPBH-UHFFFAOYSA-N

Formula: C25H52

SMILES: CCCCCCCCCCCC(CC)CCCCCCCCCC

Mol. weight [g/mol]: 352.68

CAS: 79370-85-7

Physical Properties

Property code	Value	Unit	Source
af	0.9830		Cheméo Relay (1.0)
gf	157.18	kJ/mol	Joback Method
hf	-561.17	kJ/mol	Cheméo Relay (1.0)
hfus	56.98	kJ/mol	Joback Method
hvap	118.12	kJ/mol	Cheméo Relay (1.0)
ie	9.80	eV	Cheméo Relay (1.0)
log10ws	-9.85		Cheméo Relay (1.0)
logp	9.854		Crippen Method
mcvol	363.110	ml/mol	McGowan Method
pc	767.34	kPa	Joback Method
tb	611.13	K	Cheméo Relay (1.0)
tc	779.86	K	Cheméo Relay (1.0)
tf	275.71	K	Cheméo Relay (1.0)
vc	1.415	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1258.59	J/mol×K	915.75	Joback Method
cpg	1276.97	J/mol×K	944.71	Joback Method
cpg	1175.34	J/mol×K	799.92	Joback Method
cpg	1197.69	J/mol×K	828.88	Joback Method
cpg	1218.99	J/mol×K	857.83	Joback Method
cpg	1239.27	J/mol×K	886.79	Joback Method
cpg	1151.89	J/mol×K	770.96	Joback Method

dvisc	0.0003280	Pa×s	494.66	Joback Method
dvisc	0.0007960	Pa×s	425.58	Joback Method
dvisc	0.0027240	Pa×s	356.51	Joback Method
dvisc	0.0001679	Pa×s	563.73	Joback Method
dvisc	0.0000995	Pa×s	632.81	Joback Method
dvisc	0.0000654	Pa×s	701.88	Joback Method
dvisc	0.0000463	Pa×s	770.96	Joback Method
hvapt	84.60	kJ/mol	444.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.97636e+01
Coeff. B	-1.01735e+04
Temperature range (K), min.	522.36
Temperature range (K), max.	703.94

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C79370857&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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
hvapt:	Enthalpy of vaporization at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume