3-ethyldecane

Inchi: InChI=1S/C12H26/c1-4-7-8-9-10-11-12(5-2)6-3/h12H,4-11H2,1-3H3
InchiKey: ZBDDVSBBCGZQDV-UHFFFAOYSA-N
Formula: C12H26
SMILES: CCCCCCCC(CC)CC
Mol. weight [g/mol]: 170.33
CAS: 17085-96-0

Physical Properties

Property code	Value	Unit	Source
af	0.5212		Cheméo Relay (1.0)
gf	47.72	kJ/mol	Joback Method
hf	-290.61	kJ/mol	Cheméo Relay (1.0)
hfus	23.31	kJ/mol	Joback Method
hvap	56.18	kJ/mol	Cheméo Relay (1.0)
ie	9.50	eV	Cheméo Relay (1.0)
log10ws	-6.26		Cheméo Relay (1.0)
logp	4.783		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
tb	482.00 ± 3.00	K	NIST Webbook
tb	475.20 ± 2.00	K	NIST Webbook
tc	646.83	K	Cheméo Relay (1.0)
tf	345.00 ± 4.00	K	NIST Webbook
vc	0.676	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.90	J/mol×K	473.52	Joback Method
cpg	424.06	J/mol×K	500.89	Joback Method
cpg	440.58	J/mol×K	528.26	Joback Method
cpg	456.45	J/mol×K	555.63	Joback Method
cpg	471.71	J/mol×K	583.00	Joback Method
cpg	486.36	J/mol×K	610.37	Joback Method

cpg	500.43	J/mol×K	637.74	Joback Method
dvisc	0.0101808	Pa×s	210.00	Joback Method
dvisc	0.0030132	Pa×s	253.92	Joback Method
dvisc	0.0012770	Pa×s	297.84	Joback Method
dvisc	0.0006749	Pa×s	341.76	Joback Method
dvisc	0.0004124	Pa×s	385.68	Joback Method
dvisc	0.0002787	Pa×s	429.60	Joback Method
dvisc	0.0002026	Pa×s	473.52	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42055e+01
Coeff. B	-3.74412e+03
Coeff. C	-9.13150e+01
Temperature range (K), min.	360.33
Temperature range (K), max.	512.29

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17085960&Units=SI

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

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

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
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