

1-Hentetracontene

Inchi:	InChI=1S/C41H82/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-39-41-40-38
InchiKey:	IBBOSBCTWXFHQW-UHFFFAOYSA-N
Formula:	C41H82
SMILES:	C=CC
Mol. weight [g/mol]:	575.09
CAS:	66576-37-2

Physical Properties

Property code	Value	Unit	Source
gf	382.18	kJ/mol	Joback Method
hf	-764.14	kJ/mol	Joback Method
hfus	100.67	kJ/mol	Joback Method
hvap	106.19	kJ/mol	Joback Method
log10ws	-16.84		Crippen Method
logp	16.016		Crippen Method
mcvol	584.250	ml/mol	McGowan Method
pc	382.66	kPa	Joback Method
rinpol	4096.00		NIST Webbook
tb	1134.16	K	Joback Method
tc	1529.07	K	Joback Method
tf	550.07	K	Joback Method
vc	2.312	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2214.82	J/molxK	1134.16	Joback Method
cpg	2260.52	J/molxK	1199.98	Joback Method
cpg	2302.32	J/molxK	1265.80	Joback Method
cpg	2341.06	J/molxK	1331.62	Joback Method
cpg	2377.58	J/molxK	1397.44	Joback Method
cpg	2412.73	J/molxK	1463.25	Joback Method
cpg	2447.36	J/molxK	1529.07	Joback Method
dvisc	0.0002149	Paxs	550.07	Joback Method

dvisc	0.0000700	Paxs	647.42	Joback Method
dvisc	0.0000305	Paxs	744.77	Joback Method
dvisc	0.0000161	Paxs	842.11	Joback Method
dvisc	0.0000097	Paxs	939.46	Joback Method
dvisc	0.0000065	Paxs	1036.81	Joback Method
dvisc	0.0000046	Paxs	1134.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40581e+01
Coeff. B	-5.80107e+03
Coeff. C	-2.04850e+02
Temperature range (K), min.	626.12
Temperature range (K), max.	868.08

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R628050&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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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