

nonatriacontane

Inchi: InChI=1S/C39H80/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-39-38-36-34-42
InchiKey: SNXOSZZNFRFNZ-UHFFFAOYSA-N
Formula: C39H80
SMILES: CC
Mol. weight [g/mol]: 549.05
CAS: 7194-86-7

Physical Properties

Property code	Value	Unit	Source
gf	277.50	kJ/mol	Joback Method
hf	-848.29	kJ/mol	Joback Method
hfus	96.77	kJ/mol	Joback Method
hvap	102.41	kJ/mol	Joback Method
log10ws	-16.15		Crippen Method
logp	15.460		Crippen Method
mcvol	560.370	ml/mol	McGowan Method
pc	406.15	kPa	Joback Method
tb	1091.72	K	Joback Method
tc	1442.58	K	Joback Method
tf	353.40 ± 0.60	K	NIST Webbook
tf	352.00 ± 4.00	K	NIST Webbook
tf	352.20 ± 4.00	K	NIST Webbook
vc	2.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2311.77	J/molxK	1442.58	Joback Method
cpg	2282.92	J/molxK	1384.11	Joback Method
cpg	2252.57	J/molxK	1325.63	Joback Method
cpg	2220.20	J/molxK	1267.15	Joback Method
cpg	2185.26	J/molxK	1208.67	Joback Method
cpg	2147.20	J/molxK	1150.20	Joback Method
cpg	2105.48	J/molxK	1091.72	Joback Method

dvisc	0.0002830	Paxs	529.29	Joback Method
dvisc	0.0000059	Paxs	1091.72	Joback Method
dvisc	0.0000083	Paxs	997.98	Joback Method
dvisc	0.0000125	Paxs	904.24	Joback Method
dvisc	0.0000208	Paxs	810.50	Joback Method
dvisc	0.0000395	Paxs	716.77	Joback Method
dvisc	0.0000912	Paxs	623.03	Joback Method
hvapt	130.30	kJ/mol	671.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52954e+01
Coeff. B	-6.74346e+03
Coeff. C	-1.61090e+02
Temperature range (K), min.	610.42
Temperature range (K), max.	836.52

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7194867&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvapt:	Enthalpy of vaporization at a given temperature
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

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