2-nonylnaphthalene

Inchi: InChI=1S/C19H26/c1-2-3-4-5-6-7-8-11-17-14-15-18-12-9-10-13-19(18)16-17/h9-10,12-16
InchiKey: BVGNMQMWUMKSMK-UHFFFAOYSA-N
Formula: C19H26
SMILES: CCCCCCCCCc1ccc2ccccc2c1
Mol. weight [g/mol]: 254.41
CAS: 61886-67-7

Physical Properties

Property code	Value	Unit	Source
af	0.7321		Cheméo Relay (1.0)
gf	318.53	kJ/mol	Joback Method
hf	-30.33	kJ/mol	Cheméo Relay (1.0)
hfus	35.64	kJ/mol	Joback Method
hvap	93.52	kJ/mol	Cheméo Relay (1.0)
ie	8.02	eV	Cheméo Relay (1.0)
log10ws	-7.38		Cheméo Relay (1.0)
logp	6.133		Crippen Method
mcvol	235.350	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
tb	623.00 ± 5.00	K	NIST Webbook
tc	838.45	K	Cheméo Relay (1.0)
tf	276.70 ± 3.00	K	NIST Webbook
tf	276.80 ± 1.50	K	NIST Webbook
vc	0.909	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.31	J/mol×K	684.76	Joback Method
cpg	668.95	J/mol×K	718.90	Joback Method
cpg	686.49	J/mol×K	753.03	Joback Method
cpg	703.01	J/mol×K	787.17	Joback Method
cpg	718.57	J/mol×K	821.30	Joback Method
cpg	733.25	J/mol×K	855.44	Joback Method

cpg	747.11	J/mol×K	889.58	Joback Method
dvisc	0.0016596	Pa×s	375.53	Joback Method
dvisc	0.0009354	Pa×s	427.07	Joback Method
dvisc	0.0005965	Pa×s	478.61	Joback Method
dvisc	0.0004152	Pa×s	530.14	Joback Method
dvisc	0.0003081	Pa×s	581.68	Joback Method
dvisc	0.0002401	Pa×s	633.22	Joback Method
dvisc	0.0001942	Pa×s	684.76	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43435e+01
Coeff. B	-5.06789e+03
Coeff. C	-1.19668e+02
Temperature range (K), min.	480.22
Temperature range (K), max.	680.77

Sources

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=C61886677&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):

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