

2-thiaundecane

Inchi:	InChI=1S/C10H22S/c1-3-4-5-6-7-8-9-10-11-2/h3-10H2,1-2H3
InchiKey:	FCRSULZJMFDBIK-UHFFFAOYSA-N
Formula:	C10H22S
SMILES:	CCCCCCCCCSC
Mol. weight [g/mol]:	174.35
CAS:	59973-07-8

Physical Properties

Property code	Value	Unit	Source
af	0.5090		Cheméo Relay (1.0)
gf	66.44	kJ/mol	Joback Method
hf	-221.95	kJ/mol	Cheméo Relay (1.0)
hfus	25.79	kJ/mol	Joback Method
hvap	62.42	kJ/mol	Cheméo Relay (1.0)
ie	8.57	eV	Cheméo Relay (1.0)
log10ws	-5.12		Cheméo Relay (1.0)
logp	4.100		Crippen Method
mcvol	168.110	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
tb	501.00	K	Cheméo Relay (1.0)
tc	687.59	K	Cheméo Relay (1.0)
tf	259.45	K	Cheméo Relay (1.0)
vc	0.645	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.94	J/mol×K	496.98	Joback Method
cpg	391.70	J/mol×K	527.30	Joback Method
cpg	406.81	J/mol×K	557.63	Joback Method
cpg	421.28	J/mol×K	587.95	Joback Method
cpg	435.13	J/mol×K	618.28	Joback Method
cpg	448.38	J/mol×K	648.60	Joback Method
cpg	461.02	J/mol×K	678.93	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.61956e+01
Coeff. B	-4.72184e+03
Coeff. C	-8.06670e+01
Temperature range (K), min.	377.49
Temperature range (K), max.	514.49

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor
Pressure:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C59973078&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
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

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