4-thiatridecane

Other names: nonyl propyl sulfide
Inchi: InChI=1S/C12H26S/c1-3-5-6-7-8-9-10-12-13-11-4-2/h3-12H2,1-2H3
InchiKey: AQAOPNMAEGBYHI-UHFFFAOYSA-N
Formula: C12H26S
SMILES: CCCCCCCCCSCCC
Mol. weight [g/mol]: 202.40
CAS: 62103-66-6

Physical Properties

Property code	Value	Unit	Source
af	0.5684		Cheméo Relay (1.0)
gf	83.28	kJ/mol	Joback Method
hf	-260.98	kJ/mol	Cheméo Relay (1.0)
hfus	30.97	kJ/mol	Joback Method
hvap	70.69	kJ/mol	Cheméo Relay (1.0)
ie	8.39	eV	Cheméo Relay (1.0)
log10ws	-5.87		Cheméo Relay (1.0)
logp	4.880		Crippen Method
mcvol	196.290	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
tb	527.15	K	Cheméo Relay (1.0)
tc	713.24	K	Cheméo Relay (1.0)
tf	250.57	K	Cheméo Relay (1.0)
vc	0.759	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.53	J/mol×K	542.74	Joback Method
cpg	489.74	J/mol×K	572.48	Joback Method
cpg	506.22	J/mol×K	602.21	Joback Method
cpg	521.99	J/mol×K	631.95	Joback Method
cpg	537.07	J/mol×K	661.69	Joback Method
cpg	551.47	J/mol×K	691.42	Joback Method

cpg	565.21	J/mol×K	721.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60078e+01
Coeff. B	-4.94017e+03
Coeff. C	-8.99520e+01
Temperature range (K), min.	404.21
Temperature range (K), max.	551.81

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62103666&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
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