

6-Thiatridecane

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

Physical Properties

Property code	Value	Unit	Source
gf	83.28	kJ/mol	Joback Method
hf	-249.14	kJ/mol	Joback Method
hfus	30.97	kJ/mol	Joback Method
hvap	49.12	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.880		Crippen Method
mcvol	196.290	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	1475.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1475.00		NIST Webbook
ripol	1681.00		NIST Webbook
tb	542.74	K	Joback Method
tc	721.16	K	Joback Method
tf	259.40	K	Joback Method
vc	0.761	m3/kmol	Joback Method

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	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.58200e+01
Coeff. B	-4.86493e+03
Coeff. C	-8.93960e+01
Temperature range (K), min.	402.61
Temperature range (K), max.	552.35

Sources

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=R140684&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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