

Dodecane, 1,1'-thiobis-

Other names:	Dodecyl sulfide n-Dodecyl sulfide Didodecyl sulfide Dilauryl sulfide Bis(dodecyl)sulfide Bis(n-dodecyl)sulfide NSC 12039 didodecyl sulphide
Inchi:	InChI=1S/C24H50S/c1-3-5-7-9-11-13-15-17-19-21-23-25-24-22-20-18-16-14-12-10-8-6-4
InchiKey:	UPYPTOCXMIWHSG-UHFFFAOYSA-N
Formula:	C24H50S
SMILES:	CCCCCCCCCCCCSCCCCCCCCCCCCCC
Mol. weight [g/mol]:	370.72
CAS:	2469-45-6

Physical Properties

Property code	Value	Unit	Source
gf	184.32	kJ/mol	Joback Method
hf	-496.82	kJ/mol	Joback Method
hfus	62.05	kJ/mol	Joback Method
hvap	75.84	kJ/mol	Joback Method
log10ws	-9.75		Crippen Method
logp	9.561		Crippen Method
mcvol	365.370	ml/mol	McGowan Method
pc	814.00	kPa	Joback Method
rinpol	2678.00		NIST Webbook
tb	817.30	K	Joback Method
tc	1001.47	K	Joback Method
tf	394.64	K	Joback Method
vc	1.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	1168.04	J/mol×K	817.30	Joback Method
cpg	1190.27	J/mol×K	848.00	Joback Method
cpg	1211.33	J/mol×K	878.69	Joback Method
cpg	1231.29	J/mol×K	909.39	Joback Method
cpg	1250.17	J/mol×K	940.08	Joback Method
cpg	1268.02	J/mol×K	970.78	Joback Method
cpg	1284.89	J/mol×K	1001.47	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	534.70	K	0.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2469456&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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