

Dodecyl 3-mercaptopropionate

Other names:	Dodecyl 3-mercaptopropionate Lauryl «beta»-mercaptopropionate Lauryl 3-mercaptopropionate Propionic acid, 3-mercapto-, dodecyl ester
Inchi:	InChI=1S/C15H30O2S/c1-2-3-4-5-6-7-8-9-10-11-13-17-15(16)12-14-18/h18H,2-14H2,1H
InchiKey:	ARNIBHATWCFIK-UHFFFAOYSA-N
Formula:	C15H30O2S
SMILES:	CCCCCCCCCCCCOC(=O)CCS
Mol. weight [g/mol]:	274.47

Physical Properties

Property code	Value	Unit	Source
af	0.8705		Cheméo Relay (1.0)
hf	-644.18	kJ/mol	Cheméo Relay (1.0)
hfus	41.43	kJ/mol	Joback Method
hvap	90.47	kJ/mol	Cheméo Relay (1.0)
ie	9.47	eV	Cheméo Relay (1.0)
log10ws	-5.11		Cheméo Relay (1.0)
logp	4.770		Crippen Method
mcvol	246.000	ml/mol	McGowan Method
pc	1540.29	kPa	Joback Method
tb	601.68	K	Cheméo Relay (1.0)
tc	775.32	K	Cheméo Relay (1.0)
tf	279.10	K	Cheméo Relay (1.0)
vc	0.924	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.76	J/mol×K	681.75	Joback Method
cpg	700.99	J/mol×K	712.02	Joback Method
cpg	717.40	J/mol×K	742.29	Joback Method
cpg	732.99	J/mol×K	772.56	Joback Method
cpg	747.79	J/mol×K	802.82	Joback Method

cpg	761.82	J/mol×K	833.09	Joback Method
cpg	775.09	J/mol×K	863.36	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C6380718&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

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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