

Dodecyldimethylamine oxide

Inchi:	InChI=1S/C14H31NO/c1-4-5-6-7-8-9-10-11-12-13-14-15(2,3)16/h4-14H2,1-3H3
InchiKey:	SYELZBGXAIXKHU-UHFFFAOYSA-N
Formula:	C14H31NO
SMILES:	CCCCCCCCCCCC[N+](C)(C)[O-]
Mol. weight [g/mol]:	229.41

Physical Properties

Property code	Value	Unit	Source
af	0.6930		Cheméo Relay (1.0)
gf	96.21	kJ/mol	Cheméo Relay (1.0, beta)
hf	-403.03	kJ/mol	Cheméo Relay (1.0)
hvap	84.72	kJ/mol	Cheméo Relay (1.0)
ie	8.78	eV	Cheméo Relay (1.0)
log10ws	-5.14		Cheméo Relay (1.0)
logp	4.482		Crippen Method
mcvol	223.970	ml/mol	McGowan Method
pc	1588.03	kPa	Cheméo Relay (1.0, beta)
tb	543.68	K	Cheméo Relay (1.0)
tc	714.85	K	Cheméo Relay (1.0)
tf	433.91	K	Cheméo Relay (1.0)
vc	0.854	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):	
Micellar Parameters in Solutions with Cationic Surfactants and N,N-Dimethyldodecan-1-amine Oxide: Influence of Cationic Surfactant Chain Length.	https://www.doi.org/10.1021/je201107a
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation 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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