

1-Naphthalene sulfonylchloride

Other names:	1-Naphthalenesulfonyl chloride «alpha»-Naphthalenesulfonyl chloride «alpha»-Naphthalenesulfochloride 1-Naphthylsulfonyl chloride naphthalene-1-sulphonyl chloride
Inchi:	InChI=1S/C10H7ClO2S/c11-14(12,13)10-7-3-5-8-4-1-2-6-9(8)10/h1-7H
InchiKey:	DASJFYAPNPUBGG-UHFFFAOYSA-N
Formula:	C10H7ClO2S
SMILES:	O=S(=O)(Cl)c1cccc2ccccc12
Mol. weight [g/mol]:	226.68

Physical Properties

Property code	Value	Unit	Source
af	0.5141		Cheméo Relay (1.0)
hf	-192.89	kJ/mol	Cheméo Relay (1.0)
hfus	27.90	kJ/mol	Joback Method
hvap	84.82	kJ/mol	Cheméo Relay (1.0)
ie	8.64	eV	Cheméo Relay (1.0)
log10ws	-4.12		Cheméo Relay (1.0)
logp	2.767		Crippen Method
mcvol	148.870	ml/mol	McGowan Method
pc	4450.38	kPa	Joback Method
tb	608.09	K	Cheméo Relay (1.0)
tc	904.31	K	Cheméo Relay (1.0)
tf	358.78	K	Cheméo Relay (1.0)
vc	0.526	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.56	J/mol×K	564.05	Joback Method
cpg	322.96	J/mol×K	602.99	Joback Method
cpg	334.35	J/mol×K	641.93	Joback Method
cpg	344.78	J/mol×K	680.87	Joback Method

cpg	354.30	J/mol×K	719.80	Joback Method
cpg	362.97	J/mol×K	758.74	Joback Method
cpg	370.82	J/mol×K	797.68	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85461&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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