

Nortricyclyl formate

Other names:	Nortricyclan-3-ol, formate
Inchi:	InChI=1S/C8H10O2/c9-3-10-8-4-1-5-6(2-4)7(5)8/h3-8H,1-2H2
InchiKey:	ZYRFBCPCNSLRCD-UHFFFAOYSA-N
Formula:	C8H10O2
SMILES:	O=COC1C2CC3C(C2)C31
Mol. weight [g/mol]:	138.16
CAS:	21892-95-5

Physical Properties

Property code	Value	Unit	Source
gf	2.99	kJ/mol	Joback Method
hf	-236.21	kJ/mol	Joback Method
hfus	20.70	kJ/mol	Joback Method
hvap	41.31	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	0.814		Crippen Method
mcvol	98.440	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	455.86	K	Joback Method
tc	654.47	K	Joback Method
tf	296.53	K	Joback Method
vc	0.404	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.22	J/mol×K	455.86	Joback Method
cpg	253.44	J/mol×K	488.96	Joback Method
cpg	266.67	J/mol×K	522.06	Joback Method
cpg	278.97	J/mol×K	555.16	Joback Method
cpg	290.42	J/mol×K	588.26	Joback Method
cpg	301.08	J/mol×K	621.37	Joback Method
cpg	311.04	J/mol×K	654.47	Joback Method
dvisc	0.0006153	Paxs	296.53	Joback Method

dvisc	0.0008326	Paxs	323.08	Joback Method
dvisc	0.0010760	Paxs	349.64	Joback Method
dvisc	0.0013412	Paxs	376.19	Joback Method
dvisc	0.0016239	Paxs	402.75	Joback Method
dvisc	0.0019202	Paxs	429.31	Joback Method
dvisc	0.0022266	Paxs	455.86	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	343.50 ± 0.50	K	2.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21892955&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
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
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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