

Dosulepin-M (nor-) AC

Inchi:	InChI=1S/C20H21NOS/c1-15(22)21(2)13-7-11-18-17-9-4-3-8-16(17)14-23-20-12-6-5-10-
InchiKey:	FNBUQFXNKCKNGO-WQRHYEAKSA-N
Formula:	C20H21NOS
SMILES:	CC(=O)N(C)CCC=C1c2ccccc2CSc2ccccc21
Mol. weight [g/mol]:	323.45

Physical Properties

Property code	Value	Unit	Source
gf	458.72	kJ/mol	Joback Method
hf	163.37	kJ/mol	Joback Method
hfus	40.52	kJ/mol	Joback Method
hvap	81.60	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.592		Crippen Method
mcvol	257.880	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinqol	2820.00		NIST Webbook
tb	852.51	K	Joback Method
tc	1097.29	K	Joback Method
tf	591.43	K	Joback Method
vc	0.951	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.44	J/molxK	852.51	Joback Method
cpg	764.01	J/molxK	893.31	Joback Method
cpg	778.59	J/molxK	934.10	Joback Method
cpg	792.36	J/molxK	974.90	Joback Method
cpg	805.47	J/molxK	1015.69	Joback Method
cpg	818.07	J/molxK	1056.49	Joback Method
cpg	830.34	J/molxK	1097.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R331038&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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