

Dosulepin-M (HO-) isomer-2 AC

Inchi:	InChI=1S/C21H23NO2S/c1-15(23)24-17-10-11-21-20(13-17)19(9-6-12-22(2)3)18-8-5-4-7
InchiKey:	BTXYPYZNXDAPP-OCKHKDLRSA-N
Formula:	C21H23NO2S
SMILES:	CC(=O)Oc1ccc2c(c1)C(=CCCN(C)C)c1ccccc1CS2
Mol. weight [g/mol]:	353.48

Physical Properties

Property code	Value	Unit	Source
gf	352.51	kJ/mol	Joback Method
hf	-0.96	kJ/mol	Joback Method
hfus	43.91	kJ/mol	Joback Method
hvap	86.90	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.601		Crippen Method
mvol	277.840	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	2690.00		NIST Webbook
rinpol	2690.00		NIST Webbook
tb	902.79	K	Joback Method
tc	1142.29	K	Joback Method
tf	637.45	K	Joback Method
vc	1.024	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.26	J/mol×K	902.79	Joback Method
cpg	847.43	J/mol×K	942.71	Joback Method
cpg	861.63	J/mol×K	982.62	Joback Method
cpg	874.99	J/mol×K	1022.54	Joback Method
cpg	887.62	J/mol×K	1062.46	Joback Method
cpg	899.65	J/mol×K	1102.37	Joback Method
cpg	911.22	J/mol×K	1142.29	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R331023&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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