Dosulepin-M (HO-) isomer-1 AC

Inchi: InChI=1S/C21H23NO2S/c1-15(23)24-20-12-6-10-19-18(11-7-13-22(2)3)17-9-5-4-8-16(17
InchiKey: YGZUJFGJDYILHG-WQRHYEAKSA-N
Formula: C21H23NO2S
SMILES: CC(=O)Oc1cccc2c1SCc1ccccc1C2=CCCN(C)C
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
mcvol	277.840	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	2660.00		NIST Webbook
tb	902.79	K	Joback Method
tc	1142.29	K	Joback Method
tf	637.45	K	Joback Method
vc	1.024	m3/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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R331018&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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