Dosulepin-M (nor-HO-) 2AC

Inchi: InChI=1S/C22H23NO3S/c1-15(24)23(3)12-6-9-20-19-8-5-4-7-17(19)14-27-22-11-10-18(1

InchiKey: KBHVNXXCVAKZIQ-UKWGHVSLSA-N

Formula: C22H23NO3S

SMILES: CC(=O)Oc1ccc2c(c1)C(=CCCN(C)C(C)=O)c1ccccc1CS2

Mol. weight [g/mol]: 381.49

Physical Properties

Property code	Value	Unit	Source
gf	232.01	kJ/mol	Joback Method
hf	-134.18	kJ/mol	Joback Method
hfus	48.10	kJ/mol	Joback Method
hvap	95.87	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	4.518		Crippen Method
mcvol	293.500	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
rinpol	3150.00		NIST Webbook
tb	979.54	K	Joback Method
tc	1222.51	K	Joback Method
tf	698.65	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.08	J/mol×K	979.54	Joback Method
cpg	914.85	J/mol×K	1020.03	Joback Method
cpg	927.79	J/mol×K	1060.53	Joback Method
cpg	940.01	J/mol×K	1101.02	Joback Method
cpg	951.66	J/mol×K	1141.52	Joback Method
cpg	962.87	J/mol×K	1182.01	Joback Method
cpg	973.76	J/mol×K	1222.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R331043&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

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