

Amitriptyline M(Nor-di-HO), acetylated

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C25H25NO5/c1-16(27)26(4)13-5-6-23-24-14-21(30-17(2)28)11-9-19(24)7-8-20

OEBSSXYYXMTTLO-UHFFFAOYSA-N

C25H25NO5

CC(=O)Oc1ccc2c(c1)C(=CCCN(C)C(C)=O)c1cc(OC(C)=O)ccc1C=C2

419.47

Physical Properties

Property code	Value	Unit	Source
gf	3.82	kJ/mol	Joback Method
hf	-439.85	kJ/mol	Joback Method
hfus	55.84	kJ/mol	Joback Method
hvap	106.85	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	4.321		Crippen Method
mcvol	322.560	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
tb	1080.78	K	Joback Method
tc	1326.50	K	Joback Method
tf	734.45	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1036.56	J/mol×K	1080.78	Joback Method
cpg	1048.50	J/mol×K	1121.73	Joback Method
cpg	1059.49	J/mol×K	1162.69	Joback Method
cpg	1069.63	J/mol×K	1203.64	Joback Method
cpg	1079.04	J/mol×K	1244.59	Joback Method
cpg	1087.84	J/mol×K	1285.54	Joback Method
cpg	1096.13	J/mol×K	1326.50	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R310779&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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