Melitracene M(Nor), acetylated

Inchi: InChI=1S/C22H25NO/c1-16(24)23(4)15-9-12-17-18-10-5-7-13-20(18)22(2,3)21-14-8-6-11
InchiKey: UBYPLULGKXMKSC-UHFFFAOYSA-N
Formula: C22H25NO
SMILES: CC(=O)N(C)CCC=C1c2ccccc2C(C)(C)c2ccccc21
Mol. weight [g/mol]: 319.44

Physical Properties

Property code	Value	Unit	Source
gf	434.60	kJ/mol	Joback Method
hf	77.89	kJ/mol	Joback Method
hfus	38.92	kJ/mol	Joback Method
hvap	78.61	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.626		Crippen Method
mcvol	269.710	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
rinpol	2760.00		NIST Webbook
rinpol	2760.00		NIST Webbook
tb	841.74	K	Joback Method
tc	1072.70	K	Joback Method
tf	553.70	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.75	J/mol×K	841.74	Joback Method
cpg	832.35	J/mol×K	880.23	Joback Method
cpg	850.68	J/mol×K	918.73	Joback Method
cpg	868.97	J/mol×K	957.22	Joback Method
cpg	887.47	J/mol×K	995.71	Joback Method
cpg	906.42	J/mol×K	1034.21	Joback Method
cpg	926.07	J/mol×K	1072.70	Joback Method

Sources

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=R311049&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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