Melitracene M(Nor-HO-dihydro), diacetylated

Inchi: InChI=1S/C24H29NO3/c1-16(26)25(5)14-8-10-19-20-9-6-7-11-22(20)24(3,4)23-15-18(28
InchiKey: SVWVOZFNOCWJEJ-UHFFFAOYSA-N
Formula: C24H29NO3
SMILES: CC(=O)Oc1ccc2c(c1)C(C)(C)c1ccccc1C2CCCN(C)C(C)=O
Mol. weight [g/mol]: 379.49

Physical Properties

Property code	Value	Unit	Source
gf	154.72	kJ/mol	Joback Method
hf	-316.03	kJ/mol	Joback Method
hfus	47.25	kJ/mol	Joback Method
hvap	91.78	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	4.642		Crippen Method
mcvol	309.630	ml/mol	McGowan Method
pc	1391.25	kPa	Joback Method
rinpol	3028.00		NIST Webbook
tb	957.46	K	Joback Method
tc	1186.82	K	Joback Method
tf	646.32	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1015.72	J/mol×K	957.46	Joback Method
cpg	1035.62	J/mol×K	995.69	Joback Method
cpg	1055.46	J/mol×K	1033.91	Joback Method
cpg	1075.46	J/mol×K	1072.14	Joback Method
cpg	1095.82	J/mol×K	1110.36	Joback Method
cpg	1116.76	J/mol×K	1148.59	Joback Method
cpg	1138.47	J/mol×K	1186.82	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=R311054&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