

Melitracene

Other names:	Melitracen 1-Propanamine, 3-(10,10-dimethyl-9(10H)-anthracenylidene)-N,N-dimethyl-
Inchi:	InChI=1S/C21H25N/c1-21(2)19-13-7-5-10-17(19)16(12-9-15-22(3)4)18-11-6-8-14-20(18)
InchiKey:	GWWLWDURRGNSRS-UHFFFAOYSA-N
Formula:	C21H25N
SMILES:	CN(C)CCC=C1c2ccccc2C(C)(C)c2ccccc21
Mol. weight [g/mol]:	291.43
CAS:	5118-29-6

Physical Properties

Property code	Value	Unit	Source
gf	555.10	kJ/mol	Joback Method
hf	211.11	kJ/mol	Joback Method
hfus	34.73	kJ/mol	Joback Method
hvap	69.64	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.709		Crippen Method
mcvol	254.050	ml/mol	McGowan Method
pc	1700.50	kPa	Joback Method
rinpol	2295.00		NIST Webbook
rinpol	2326.00		NIST Webbook
rinpol	2285.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2285.00		NIST Webbook
tb	764.99	K	Joback Method
tc	993.97	K	Joback Method
tf	492.50	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.80	J/molxK	764.99	Joback Method
cpg	755.88	J/molxK	803.15	Joback Method

cpg	774.30	J/mol×K	841.32	Joback Method
cpg	792.28	J/mol×K	879.48	Joback Method
cpg	810.08	J/mol×K	917.64	Joback Method
cpg	827.92	J/mol×K	955.81	Joback Method
cpg	846.04	J/mol×K	993.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5118296&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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