

Phenanthrene, 3,9-bis(1,1-dimethylethyl)-

Inchi:	InChI=1S/C22H26/c1-21(2,3)16-12-11-15-13-20(22(4,5)6)18-10-8-7-9-17(18)19(15)14-16
InchiKey:	UENRPNPQJZVMPN-UHFFFAOYSA-N
Formula:	C22H26
SMILES:	CC(C)(C)c1ccc2cc(C(C)(C)C)c3ccccc3c2c1
Mol. weight [g/mol]:	290.44
CAS:	55125-03-6

Physical Properties

Property code	Value	Unit	Source
gf	436.86	kJ/mol	Joback Method
hf	69.35	kJ/mol	Joback Method
hfus	24.82	kJ/mol	Joback Method
hvap	69.52	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	6.588		Crippen Method
mcvol	258.160	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
tb	775.88	K	Joback Method
tc	1017.59	K	Joback Method
tf	471.92	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.14	J/molxK	775.88	Joback Method
cpg	774.91	J/molxK	816.16	Joback Method
cpg	792.47	J/molxK	856.45	Joback Method
cpg	808.99	J/molxK	896.73	Joback Method
cpg	824.69	J/molxK	937.02	Joback Method
cpg	839.76	J/molxK	977.30	Joback Method
cpg	854.40	J/molxK	1017.59	Joback Method
dvisc	0.0010875	Paxs	471.92	Joback Method
dvisc	0.0006996	Paxs	522.58	Joback Method

dvisc	0.0004865	Paxs	573.24	Joback Method
dvisc	0.0003589	Paxs	623.90	Joback Method
dvisc	0.0002772	Paxs	674.56	Joback Method
dvisc	0.0002219	Paxs	725.22	Joback Method
dvisc	0.0001829	Paxs	775.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55125036&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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