9-Methyl triptycene

Inchi: InChI=1S/C21H16/c1-21-17-11-5-2-8-14(17)20(15-9-3-6-12-18(15)21)16-10-4-7-13-19(16
InchiKey: OFWMYJWQNDGHLY-UHFFFAOYSA-N
Formula: C21H16
SMILES: CC12c3ccccc3C(c3ccccc31)c1ccccc12
Mol. weight [g/mol]: 268.35
CAS: 793-39-5

Physical Properties

Property code	Value	Unit	Source
gf	598.69	kJ/mol	Joback Method
hf	383.89	kJ/mol	Joback Method
hfus	29.47	kJ/mol	Joback Method
hvap	69.14	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.848		Crippen Method
mcvol	213.750	ml/mol	McGowan Method
pc	2309.17	kPa	Joback Method
tb	771.50	K	Joback Method
tc	1035.45	K	Joback Method
tf	517.11	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.40	J/mol×K	771.50	Joback Method
cpg	623.60	J/mol×K	815.49	Joback Method
cpg	640.52	J/mol×K	859.48	Joback Method
cpg	657.59	J/mol×K	903.47	Joback Method
cpg	675.26	J/mol×K	947.46	Joback Method
cpg	693.94	J/mol×K	991.46	Joback Method
cpg	714.10	J/mol×K	1035.45	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=C793395&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume