1-Phenyl-2-(3-phenathryl)ethylene, trans

Inchi: InChI=1S/C22H16/c1-2-6-17(7-3-1)10-11-18-12-13-20-15-14-19-8-4-5-9-21(19)22(20)16-
InchiKey: RNUWWCWTCAKZTI-ZHACJKMWSA-N
Formula: C22H16
SMILES: C(=Cc1ccc2ccc3ccccc3c2c1)c1ccccc1
Mol. weight [g/mol]: 280.36

Physical Properties

Property code	Value	Unit	Source
gf	633.44	kJ/mol	Joback Method
hf	452.07	kJ/mol	Joback Method
hfus	34.28	kJ/mol	Joback Method
hvap	73.68	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	6.163		Crippen Method
mcvol	230.100	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	2915.00		NIST Webbook
rinpol	2915.00		NIST Webbook
rinpol	2975.00		NIST Webbook
rinpol	2975.00		NIST Webbook
tb	808.20	K	Joback Method
tc	1075.85	K	Joback Method
tf	475.90	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.16	J/mol×K	808.20	Joback Method
cpg	708.26	J/mol×K	1031.24	Joback Method
cpg	695.07	J/mol×K	986.63	Joback Method
cpg	681.51	J/mol×K	942.03	Joback Method
cpg	667.34	J/mol×K	897.42	Joback Method
cpg	652.30	J/mol×K	852.81	Joback Method

cpg	721.33	J/mol×K	1075.85	Joback Method
dvisc	0.0002565	Pa×s	808.20	Joback Method
dvisc	0.0003001	Pa×s	752.82	Joback Method
dvisc	0.0003601	Pa×s	697.43	Joback Method
dvisc	0.0004459	Pa×s	642.05	Joback Method
dvisc	0.0005748	Pa×s	586.67	Joback Method
dvisc	0.0007813	Pa×s	531.28	Joback Method
dvisc	0.0011407	Pa×s	475.90	Joback Method

Sources

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=R525278&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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