2,7-dimethylpyrene

Other names: Pyrene, 2,7-dimethyl-
Inchi: InChI=1S/C18H14/c1-11-7-13-3-5-15-9-12(2)10-16-6-4-14(8-11)17(13)18(15)16/h3-10H,
InchiKey: GSKHIRFMTJUBSM-UHFFFAOYSA-N
Formula: C18H14
SMILES: Cc1cc2ccc3cc(C)cc4ccc(c1)c2c34
Mol. weight [g/mol]: 230.30
CAS: 15679-24-0

Physical Properties

Property code	Value	Unit	Source
gf	488.76	kJ/mol	Joback Method
hf	303.55	kJ/mol	Joback Method
hfus	28.90	kJ/mol	Joback Method
hvap	64.87	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	5.201		Crippen Method
mcvol	186.640	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	386.96		NIST Webbook
rinpol	386.34		NIST Webbook
rinpol	386.34		NIST Webbook
rinpol	387.00		NIST Webbook
rinpol	387.00		NIST Webbook
tb	707.08	K	Joback Method
tc	953.50	K	Joback Method
tf	473.50	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.24	J/mol×K	707.08	Joback Method
cpg	499.40	J/mol×K	748.15	Joback Method
cpg	512.64	J/mol×K	789.22	Joback Method

cpg	525.12	J/mol×K	830.29	Joback Method
cpg	537.04	J/mol×K	871.36	Joback Method
cpg	548.57	J/mol×K	912.43	Joback Method
cpg	559.89	J/mol×K	953.50	Joback Method
dvisc	0.0019651	Pa×s	473.50	Joback Method
dvisc	0.0017819	Pa×s	512.43	Joback Method
dvisc	0.0016382	Pa×s	551.36	Joback Method
dvisc	0.0015229	Pa×s	590.29	Joback Method
dvisc	0.0014286	Pa×s	629.22	Joback Method
dvisc	0.0013501	Pa×s	668.15	Joback Method
dvisc	0.0012839	Pa×s	707.08	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=C15679240&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