Pyrene, 1-ethyl-

Other names: 1-ethylpyrene
Inchi: InChI=1S/C18H14/c1-2-12-6-7-15-9-8-13-4-3-5-14-10-11-16(12)18(15)17(13)14/h3-11H,
InchiKey: ZWAMZDRREBOHIO-UHFFFAOYSA-N
Formula: C18H14
SMILES: CCc1ccc2ccc3cccc4ccc1c2c34
Mol. weight [g/mol]: 230.30
CAS: 17088-22-1

Physical Properties

Property code	Value	Unit	Source
gf	498.39	kJ/mol	Joback Method
hf	315.02	kJ/mol	Joback Method
hfus	29.29	kJ/mol	Joback Method
hvap	64.21	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	5.146		Crippen Method
mcvol	186.640	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
rinpol	386.60		NIST Webbook
rinpol	385.35		NIST Webbook
rinpol	385.35		NIST Webbook
rinpol	385.02		NIST Webbook
rinpol	385.35		NIST Webbook
rinpol	385.02		NIST Webbook
rinpol	385.35		NIST Webbook
tb	702.10	K	Joback Method
tc	947.69	K	Joback Method
tf	365.65 ± 2.00	K	NIST Webbook
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.49	J/mol×K	702.10	Joback Method

cpg	550.08	J/mol×K	906.76	Joback Method
cpg	538.57	J/mol×K	865.83	Joback Method
cpg	526.65	J/mol×K	824.90	Joback Method
cpg	514.11	J/mol×K	783.96	Joback Method
cpg	500.79	J/mol×K	743.03	Joback Method
cpg	561.35	J/mol×K	947.69	Joback Method
dvisc	0.0012650	Pa×s	702.10	Joback Method
dvisc	0.0013394	Pa×s	661.91	Joback Method
dvisc	0.0014288	Pa×s	621.73	Joback Method
dvisc	0.0015378	Pa×s	581.54	Joback Method
dvisc	0.0016732	Pa×s	541.35	Joback Method
dvisc	0.0018454	Pa×s	501.17	Joback Method
dvisc	0.0020704	Pa×s	460.98	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=C17088221&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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