Benz[a]anthracene, 8-propyl-

Other names: 5-n-Propyl-1,2-benzanthracene
Inchi: InChI=1S/C21H18/c1-2-6-15-8-5-9-17-14-21-18(13-20(15)17)12-11-16-7-3-4-10-19(16)21
InchiKey: MUVMFAXETLUFCG-UHFFFAOYSA-N
Formula: C21H18
SMILES: CCCc1cccc2cc3c(ccc4ccccc43)cc12
Mol. weight [g/mol]: 270.37
CAS: 54889-82-6

Physical Properties

Property code	Value	Unit	Source
gf	529.41	kJ/mol	Joback Method
hf	298.56	kJ/mol	Joback Method
hfus	34.08	kJ/mol	Joback Method
hvap	71.52	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	6.099		Crippen Method
mcvol	224.610	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
tb	778.44	K	Joback Method
tc	1025.53	K	Joback Method
tf	488.51	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.15	J/mol×K	778.44	Joback Method
cpg	697.86	J/mol×K	984.35	Joback Method
cpg	684.79	J/mol×K	943.17	Joback Method
cpg	671.27	J/mol×K	901.98	Joback Method
cpg	657.11	J/mol×K	860.80	Joback Method
cpg	642.13	J/mol×K	819.62	Joback Method
cpg	710.65	J/mol×K	1025.53	Joback Method
dvisc	0.0005994	Pa×s	778.44	Joback Method

dvisc	0.0006680	Pa×s	730.12	Joback Method
dvisc	0.0007560	Pa×s	681.80	Joback Method
dvisc	0.0008719	Pa×s	633.48	Joback Method
dvisc	0.0010295	Pa×s	585.15	Joback Method
dvisc	0.0012525	Pa×s	536.83	Joback Method
dvisc	0.0015842	Pa×s	488.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54889826&Units=SI
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

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