ACENAPHTHO[1,2-J]FLUORANTHENE

Inchi: InChI=1S/C26H14/c1-5-15-7-3-11-21-23(15)17(9-1)19-13-14-20-18-10-2-6-16-8-4-12-22(
InchiKey: ILYGRCGTUMHLGR-UHFFFAOYSA-N
Formula: C26H14
SMILES: c1cc2cccc3c2c(c1)c1ccc2c4cccc5cccc(c54)c2c13
Mol. weight [g/mol]: 326.40

Physical Properties

Property code	Value	Unit	Source
hf	442.58	kJ/mol	Cheméo Relay (1.0)
hfus	43.26	kJ/mol	Joback Method
hvap	157.94	kJ/mol	Cheméo Relay (1.0)
ie	6.83	eV	Cheméo Relay (1.0)
log10ws	-10.13		Cheméo Relay (1.0)
logp	7.481		Crippen Method
mcvol	245.280	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
tb	869.55	K	Cheméo Relay (1.0)
tc	1235.12	K	Cheméo Relay (1.0)
tf	555.78	K	Cheméo Relay (1.0)
vc	0.991	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.27	J/mol×K	944.34	Joback Method
cpg	839.08	J/mol×K	1213.26	Joback Method
cpg	813.43	J/mol×K	1168.44	Joback Method
cpg	790.49	J/mol×K	1123.62	Joback Method
cpg	769.83	J/mol×K	1078.80	Joback Method
cpg	751.03	J/mol×K	1033.98	Joback Method
cpg	733.65	J/mol×K	989.16	Joback Method
dvisc	0.0151603	Pa×s	812.45	Joback Method
dvisc	0.0149317	Pa×s	944.34	Joback Method
dvisc	0.0150001	Pa×s	900.38	Joback Method

dvisc	0.0150758	Pa×s	856.41	Joback Method
dvisc	0.0154834	Pa×s	680.56	Joback Method
dvisc	0.0152550	Pa×s	768.49	Joback Method
dvisc	0.0153618	Pa×s	724.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C193215&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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