NAPHTHO[2,1,8-FGH]PENTAPHENE

Inchi: InChI=1S/C28H16/c1-2-7-19-15-25-24(14-18(19)6-1)22-11-5-9-17-12-13-23-21-10-4-3-8-
InchiKey: GWQNZHNLKCYFOP-UHFFFAOYSA-N
Formula: C28H16
SMILES: c1ccc2cc3c(cc2c1)c1cccc2ccc4c5ccccc5cc3c4c21
Mol. weight [g/mol]: 352.44

Physical Properties

Property code	Value	Unit	Source
hf	473.99	kJ/mol	Cheméo Relay (1.0)
hfus	45.46	kJ/mol	Joback Method
hvap	167.40	kJ/mol	Cheméo Relay (1.0)
ie	6.87	eV	Cheméo Relay (1.0)
log10ws	-10.91		Cheméo Relay (1.0)
logp	8.044		Crippen Method
mcvol	269.160	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
tb	905.17	K	Cheméo Relay (1.0)
tc	1274.25	K	Cheméo Relay (1.0)
tf	574.64	K	Cheméo Relay (1.0)
vc	1.052	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.33	J/mol×K	997.80	Joback Method
cpg	830.69	J/mol×K	1043.48	Joback Method
cpg	850.20	J/mol×K	1089.16	Joback Method
cpg	871.30	J/mol×K	1134.83	Joback Method
cpg	894.41	J/mol×K	1180.51	Joback Method
cpg	919.98	J/mol×K	1226.19	Joback Method
cpg	948.44	J/mol×K	1271.87	Joback Method
dvisc	0.0086256	Pa×s	696.82	Joback Method
dvisc	0.0081349	Pa×s	746.98	Joback Method
dvisc	0.0077289	Pa×s	797.15	Joback Method

dvisc	0.0073878	Pa×s	847.31	Joback Method
dvisc	0.0070975	Pa×s	897.47	Joback Method
dvisc	0.0068476	Pa×s	947.64	Joback Method
dvisc	0.0066304	Pa×s	997.80	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19301883&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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