[4.2.2]PROPELLA-2,4,7,9-TETRAENE

Inchi: InChI=1S/C10H8/c1-2-4-10-7-5-9(10,3-1)6-8-10/h1-8H
InchiKey: HLHKYPRYFGATQL-UHFFFAOYSA-N
Formula: C10H8
SMILES: C1=CC23C=CC2(C=C1)C=C3
Mol. weight [g/mol]: 128.17

Physical Properties

Property code	Value	Unit	Source
hfus	5.18	kJ/mol	Joback Method
ie	8.06	eV	NIST Webbook
logp	2.225		Crippen Method
mcvol	101.980	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.76	J/mol×K	454.48	Joback Method
cpg	229.19	J/mol×K	495.28	Joback Method
cpg	242.31	J/mol×K	536.08	Joback Method
cpg	253.54	J/mol×K	576.88	Joback Method
cpg	263.28	J/mol×K	617.67	Joback Method
cpg	271.96	J/mol×K	658.47	Joback Method
cpg	279.99	J/mol×K	699.27	Joback Method

Sources

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
Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C88090340&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume