

dihydrochrysene

Inchi:	InChI=1S/C18H14/c1-3-7-15-13(5-1)9-11-18-16-8-4-2-6-14(16)10-12-17(15)18/h1-9,11H
InchiKey:	QAOVZIXGCXUFMK-UHFFFAOYSA-N
Formula:	C18H14
SMILES:	<chem>c1ccc2c(c1)CCc1c-2ccc2ccccc12</chem>
Mol. weight [g/mol]:	230.30
CAS:	41593-31-1

Physical Properties

Property code	Value	Unit	Source
gf	483.82	kJ/mol	Joback Method
hf	314.17	kJ/mol	Joback Method
hfus	25.47	kJ/mol	Joback Method
hvap	63.89	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	4.605		Crippen Method
mvol	186.640	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
rinpol	2328.80		NIST Webbook
tb	705.66	K	Joback Method
tc	966.71	K	Joback Method
tf	441.42	K	Joback Method
vc	0.716	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.22	J/molxK	705.66	Joback Method
cpg	508.26	J/molxK	749.17	Joback Method
cpg	523.03	J/molxK	792.68	Joback Method
cpg	536.73	J/molxK	836.19	Joback Method
cpg	549.58	J/molxK	879.70	Joback Method
cpg	561.76	J/molxK	923.20	Joback Method
cpg	573.50	J/molxK	966.71	Joback Method
dvisc	0.0017899	Paxs	441.42	Joback Method

dvisc	0.0014163	Paxs	485.46	Joback Method
dvisc	0.0011651	Paxs	529.50	Joback Method
dvisc	0.0009877	Paxs	573.54	Joback Method
dvisc	0.0008572	Paxs	617.58	Joback Method
dvisc	0.0007582	Paxs	661.62	Joback Method
dvisc	0.0006809	Paxs	705.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41593311&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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