Chrysene, 6-octyl-

Other names: 6-n-Octylchrysene
6-octylchrysene
Inchi: InChI=1S/C26H28/c1-2-3-4-5-6-7-13-21-19-26-22-14-9-8-12-20(22)17-18-25(26)24-16-1
InchiKey: KTSUECCHGKCKHX-UHFFFAOYSA-N
Formula: C26H28
SMILES: CCCCCCCCc1cc2c3ccccc3ccc2c2ccccc12
Mol. weight [g/mol]: 340.50
CAS: 56248-66-9

Physical Properties

Property code	Value	Unit	Source
gf	571.51	kJ/mol	Joback Method
hf	195.36	kJ/mol	Joback Method
hfus	47.03	kJ/mol	Joback Method
hvap	82.65	kJ/mol	Joback Method
log10ws	-10.20		Crippen Method
logp	8.049		Crippen Method
mcvol	295.060	ml/mol	McGowan Method
pc	1378.88	kPa	Joback Method
tb	892.84	K	Joback Method
tc	1122.29	K	Joback Method
tf	544.86	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	913.26	J/mol×K	892.84	Joback Method
cpg	995.25	J/mol×K	1084.05	Joback Method
cpg	979.69	J/mol×K	1045.81	Joback Method
cpg	963.87	J/mol×K	1007.57	Joback Method
cpg	947.64	J/mol×K	969.32	Joback Method
cpg	930.82	J/mol×K	931.08	Joback Method
cpg	1010.72	J/mol×K	1122.29	Joback Method

dvisc	0.0003834	Pa×s	892.84	Joback Method
dvisc	0.0004391	Pa×s	834.84	Joback Method
dvisc	0.0005133	Pa×s	776.85	Joback Method
dvisc	0.0006154	Pa×s	718.85	Joback Method
dvisc	0.0007615	Pa×s	660.85	Joback Method
dvisc	0.0009818	Pa×s	602.86	Joback Method
dvisc	0.0013363	Pa×s	544.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56248669&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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