8b,16b-Dihydrodibenzo[g,p]chrysene mixture of cis and trans

Inchi: InChI=1S/C26H18/c1-5-13-21-17(9-1)18-10-2-6-14-22(18)26-24-16-8-4-12-20(24)19-11-3

InchiKey: BUBKFBKPMDZRIJ-UHFFFAOYSA-N

Formula: C26H18

SMILES: c1ccc2c(c1)-c1ccccc1C1c3ccccc3-c3ccccc3C21

Mol. weight [g/mol]: 330.42

CAS: 33741-19-4

Physical Properties

Property code	Value	Unit	Source
chs	-13178.00	kJ/mol	NIST Webbook
gf	749.06	kJ/mol	Joback Method
hf	490.51	kJ/mol	Joback Method
hfus	42.37	kJ/mol	Joback Method
hsub	182.00	kJ/mol	NIST Webbook
hvap	84.36	kJ/mol	Joback Method
log10ws	-8.95		Crippen Method
logp	6.611		Crippen Method
mcvol	260.440	ml/mol	McGowan Method
pc	1906.90	kPa	Joback Method
tb	917.32	K	Joback Method
tc	1188.78	K	Joback Method
tf	588.50	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.71	J/mol×K	917.32	Joback Method
cpg	812.87	J/mol×K	962.56	Joback Method
cpg	829.68	J/mol×K	1007.81	Joback Method
cpg	846.48	J/mol×K	1053.05	Joback Method
cpg	863.61	J/mol×K	1098.29	Joback Method
cpg	881.43	J/mol×K	1143.53	Joback Method
cpg	900.26	J/mol×K	1188.78	Joback Method

dvisc	0.0042000	Pa×s	588.50	Joback Method
dvisc	0.0037395	Pa×s	643.30	Joback Method
dvisc	0.0033909	Pa×s	698.11	Joback Method
dvisc	0.0031188	Pa×s	752.91	Joback Method
dvisc	0.0029013	Pa×s	807.71	Joback Method
dvisc	0.0027239	Pa×s	862.52	Joback Method
dvisc	0.0025767	Pa×s	917.32	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33741194&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
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
hsub:	Enthalpy of sublimation 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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