

Benz[def]indeno[1,2,3-qr]chrysene

Inchi:	InChI=1S/C26H14/c1-2-6-18-16(5-1)13-17-10-9-15-11-12-21-19-7-3-4-8-20(19)23-14-22
InchiKey:	FSUPSEJFXMSVMS-UHFFFAOYSA-N
Formula:	C26H14
SMILES:	<chem>c1ccc2c(c1)-c1ccc3ccc4cc5ccccc5c5cc-2c1c3c45</chem>
Mol. weight [g/mol]:	326.39
CAS:	111189-34-5

Physical Properties

Property code	Value	Unit	Source
gf	860.68	kJ/mol	Joback Method
hf	654.71	kJ/mol	Joback Method
hfus	43.26	kJ/mol	Joback Method
hvap	87.62	kJ/mol	Joback Method
log10ws	-11.56		Crippen Method
logp	7.385		Crippen Method
mvol	245.280	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
tb	944.34	K	Joback Method
tc	1213.26	K	Joback Method
tf	680.56	K	Joback Method
vc	0.976	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.27	J/molxK	944.34	Joback Method
cpg	733.65	J/molxK	989.16	Joback Method
cpg	751.03	J/molxK	1033.98	Joback Method
cpg	769.83	J/molxK	1078.80	Joback Method
cpg	790.49	J/molxK	1123.62	Joback Method
cpg	813.43	J/molxK	1168.44	Joback Method
cpg	839.08	J/molxK	1213.26	Joback Method
dvisc	0.0154834	Paxs	680.56	Joback Method
dvisc	0.0153618	Paxs	724.52	Joback Method

dvisc	0.0152550	Paxs	768.49	Joback Method
dvisc	0.0151603	Paxs	812.45	Joback Method
dvisc	0.0150758	Paxs	856.41	Joback Method
dvisc	0.0150001	Paxs	900.38	Joback Method
dvisc	0.0149317	Paxs	944.34	Joback Method

Sources

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=C111189345&Units=SI
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
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
mccvol:	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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