Benzo[1,2,3-cd:4,5,6-c'd']diperylene

Other names: Benzo(1,2,3-cd;4,5,6-c'd')diperylene
Inchi: InChI=1S/C40H20/c1-5-21-6-2-10-24-28-14-18-32-34-20-16-30-26-12-4-8-22-7-3-11-25(
InchiKey: GGVMPKQSTZIOIU-UHFFFAOYSA-N
Formula: C40H20
SMILES: c1cc2cccc3c4ccc5c6ccc7c8cccc9cccc(c%10ccc(c%11ccc(c(c1)c23)c4c%115)c6c%107)c
Mol. weight [g/mol]: 500.59
CAS: 188-73-8

Physical Properties

Property code	Value	Unit	Source
gf	1360.88	kJ/mol	Joback Method
hf	1038.69	kJ/mol	Joback Method
hfus	69.02	kJ/mol	Joback Method
hvap	127.36	kJ/mol	Joback Method
ie	6.11 ± 0.02	eV	NIST Webbook
log10ws	-17.76		Crippen Method
logp	11.532		Crippen Method
mcvol	369.000	ml/mol	McGowan Method
pc	1402.74	kPa	Joback Method
tb	1352.80	K	Joback Method
tc	1658.35	K	Joback Method
tf	1025.50	K	Joback Method
vc	1.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1430.84	J/mol×K	1352.80	Joback Method
cpg	1505.77	J/mol×K	1403.73	Joback Method
cpg	1590.95	J/mol×K	1454.65	Joback Method
cpg	1687.35	J/mol×K	1505.58	Joback Method
cpg	1795.97	J/mol×K	1556.50	Joback Method
cpg	1917.79	J/mol×K	1607.43	Joback Method
cpg	2053.80	J/mol×K	1658.35	Joback Method

dvisc	0.3335825	Pa×s	1025.50	Joback Method
dvisc	0.3388752	Pa×s	1080.05	Joback Method
dvisc	0.3437312	Pa×s	1134.60	Joback Method
dvisc	0.3482019	Pa×s	1189.15	Joback Method
dvisc	0.3523311	Pa×s	1243.70	Joback Method
dvisc	0.3561563	Pa×s	1298.25	Joback Method
dvisc	0.3597096	Pa×s	1352.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C188738&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
ie:	Ionization energy
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