Tribenzo[de,h,kl]naphtho[1,2,3,4-rst]tetraphene

Inchi: InChI=1S/C38H20/c1-2-14-24-23(13-1)33-27-17-5-9-21-10-7-19-29(31(21)27)35-25-15-3
InchiKey: SZPCSERRBCRIJE-UHFFFAOYSA-N
Formula: C38H20
SMILES: c1ccc2c(c1)c1c3cccc4cccc(c43)c3c4ccccc4c4c5cccc6cccc(c65)c2c4c13
Mol. weight [g/mol]: 476.57
CAS: 187-96-2

Physical Properties

Property code	Value	Unit	Source
gf	1252.78	kJ/mol	Joback Method
hf	945.83	kJ/mol	Joback Method
hfus	64.23	kJ/mol	Joback Method
hvap	121.24	kJ/mol	Joback Method
ie	6.06 ± 0.02	eV	NIST Webbook
ie	6.06 ± 0.02	eV	NIST Webbook
log10ws	-16.54		Crippen Method
logp	10.941		Crippen Method
mcvol	355.980	ml/mol	McGowan Method
pc	1454.57	kPa	Joback Method
tb	1290.78	K	Joback Method
tc	1587.53	K	Joback Method
tf	951.46	K	Joback Method
vc	1.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1289.31	J/mol×K	1290.78	Joback Method
cpg	1343.28	J/mol×K	1340.24	Joback Method
cpg	1404.48	J/mol×K	1389.70	Joback Method
cpg	1473.71	J/mol×K	1439.16	Joback Method
cpg	1551.77	J/mol×K	1488.62	Joback Method
cpg	1639.46	J/mol×K	1538.07	Joback Method
cpg	1737.61	J/mol×K	1587.53	Joback Method

dvisc	0.0838487	Pa×s	951.46	Joback Method
dvisc	0.0830033	Pa×s	1008.01	Joback Method
dvisc	0.0822549	Pa×s	1064.57	Joback Method
dvisc	0.0815878	Pa×s	1121.12	Joback Method
dvisc	0.0809894	Pa×s	1177.67	Joback Method
dvisc	0.0804497	Pa×s	1234.23	Joback Method
dvisc	0.0799604	Pa×s	1290.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C187962&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