1,3,5-Tri-2-naphthylbenzene

Inchi: InChI=1S/C36H24/c1-4-10-28-19-31(16-13-25(28)7-1)34-22-35(32-17-14-26-8-2-5-11-29
InchiKey: AWIOMAWDKDFGDP-UHFFFAOYSA-N
Formula: C36H24
SMILES: c1ccc2cc(-c3cc(-c4ccc5ccccc5c4)cc(-c4ccc5ccccc5c4)c3)ccc2c1
Mol. weight [g/mol]: 456.58
CAS: 7059-70-3

Physical Properties

Property code	Value	Unit	Source
gf	973.68	kJ/mol	Joback Method
hf	675.61	kJ/mol	Joback Method
hfus	54.27	kJ/mol	Joback Method
hvap	113.06	kJ/mol	Joback Method
log10ws	-14.69		Crippen Method
logp	10.147		Crippen Method
mcvol	364.680	ml/mol	McGowan Method
pc	1381.96	kPa	Joback Method
tb	1211.64	K	Joback Method
tc	1507.41	K	Joback Method
tf	761.86	K	Joback Method
vc	1.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1205.28	J/mol×K	1211.64	Joback Method
cpg	1227.37	J/mol×K	1260.94	Joback Method
cpg	1250.81	J/mol×K	1310.23	Joback Method
cpg	1276.06	J/mol×K	1359.53	Joback Method
cpg	1303.59	J/mol×K	1408.82	Joback Method
cpg	1333.85	J/mol×K	1458.12	Joback Method
cpg	1367.30	J/mol×K	1507.41	Joback Method
cps	481.00	J/mol×K	300.00	NIST Webbook
dvisc	0.0004206	Pa×s	836.82	Joback Method

dvisc	0.0005768	Pa×s	761.86	Joback Method
dvisc	0.0003231	Pa×s	911.79	Joback Method
dvisc	0.0002583	Pa×s	986.75	Joback Method
dvisc	0.0002132	Pa×s	1061.71	Joback Method
dvisc	0.0001804	Pa×s	1136.68	Joback Method
dvisc	0.0001559	Pa×s	1211.64	Joback Method
hfust	42.26	kJ/mol	472.00	NIST Webbook
hfust	42.42	kJ/mol	472.00	NIST Webbook
sfust	89.90	J/mol×K	472.00	NIST Webbook

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=C7059703&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume