(1«alpha»,2«alpha»,3«beta»,6«beta»)-1,2,3,6-tetra anhydride

Othernames: exo-5-norbornene-2,3-dicarboxylic anhydride
Inchi: InChI=1S/C9H8O3/c10-8-6-4-1-2-5(3-4)7(6)9(11)12-8/h1-2,4-7H,3H2/t4-,5-,6-,7+/m1/s1
InchiKey: KNDQHSIWLOJIGP-GBNDHIKLSA-N
Formula: C9H8O3
SMILES: O=C1OC(=O)C2C3C=CC(C3)C12
Mol. weight [g/mol]: 164.16
CAS: 2746-19-2

Physical Properties

Property code	Value	Unit	Source
gf	-114.00	kJ/mol	Joback Method
hf	-386.81	kJ/mol	Joback Method
hfus	20.66	kJ/mol	Joback Method
hvap	48.53	kJ/mol	Joback Method
log10ws	-0.80		Crippen Method
logp	0.508		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
pc	3891.64	kPa	Joback Method
tb	586.89	K	Joback Method
tc	837.54	K	Joback Method
tf	401.02	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.29	J/mol×K	753.99	Joback Method
cpg	372.95	J/mol×K	795.77	Joback Method
cpg	304.71	J/mol×K	586.89	Joback Method
cpg	320.44	J/mol×K	628.67	Joback Method
cpg	335.09	J/mol×K	670.44	Joback Method
cpg	348.69	J/mol×K	712.22	Joback Method
cpg	383.70	J/mol×K	837.54	Joback Method
hfust	21.77	kJ/mol	416.20	NIST Webbook

hfust	21.77	kJ/mol	416.20	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2746192&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

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume