Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 2-[3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-

Other names:	Irganox 1024
	2,3-bis[[3-[3,5-di-tert-butyl-4-hydroxyphenyl]propionyl]]propionohydrazide
	N,N'-bis[3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionyl]hydrazine
Inchi:	InChI=1S/C34H52N2O4/c1-31(2,3)23-17-21(18-24(29(23)39)32(4,5)6)13-15-27(37)35-36
InchiKey:	HCILJBJJZALOAL-UHFFFAOYSA-N
Formula:	C34H52N2O4
SMILES:	CC(C)(C)c1cc(CCC(=O)NNC(=O)CCc2cc(C(C)(C)C)c(O)c(C(C)(C)C)c2)cc(C(C)(C)C)c1O
Mol. weight [g/mol]:	552.79
CAS:	32687-78-8

Physical Properties

Property code	Value	Unit	Source
gf	44.76	kJ/mol	Joback Method
hf	-825.75	kJ/mol	Joback Method
hfus	65.65	kJ/mol	Joback Method
hvap	145.69	kJ/mol	Joback Method
log10ws	-8.83		Crippen Method
logp	7.001		Crippen Method
mcvol	477.240	ml/mol	McGowan Method
pc	888.94	kPa	Joback Method
tb	1407.00	K	Joback Method
tc	1753.11	K	Joback Method
tf	1014.16	K	Joback Method
vc	1.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1940.17	J/mol×K	1407.00	Joback Method
cpg	2000.96	J/mol×K	1464.68	Joback Method
cpg	2068.95	J/mol×K	1522.37	Joback Method
cpg	2145.18	J/mol×K	1580.05	Joback Method
cpg	2230.68	J/mol×K	1637.74	Joback Method
cpg	2326.49	J/mol×K	1695.42	Joback Method

cpg	2433.66	J/mol×K	1753.11	Joback Method
hfust	41.50	kJ/mol	503.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32687788&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