Carbosulfan

Other names:	Carbamic acid, [(dibutylamino)thio]methyl-, 2,3-dihydro-2,2-dimethyl-7-benzofuranyl ester
	2,3-Dihydro-2,2-dimethyl-7-benzofuranyl[(dibutylamino)thio]methyl carbamate
	Advantage
	FMC 35001
	Marshal
	OMS 3022
	Posse
	Sheriff
	2,3-dihydro-2,2-dimethyl-7-benzofuryl [(dibutylamino)thio]methylcarbamate
Inchi:	InChI=1S/C20H32N2O3S/c1-6-8-13-22(14-9-7-2)26-21(5)19(23)24-17-12-10-11-16-15-2(
InchiKey:	JLQUFIHWVLZVTJ-UHFFFAOYSA-N
Formula:	C20H32N2O3S
SMILES:	CCCCN(CCCC)SN(C)C(=O)Oc1cccc2c1OC(C)(C)C2
Mol. weight [g/mol]:	380.55
CAS:	55285-14-8

Physical Properties

Property code	Value	Unit	Source
gf	200.57	kJ/mol	Joback Method
hf	-354.37	kJ/mol	Joback Method
hfus	53.59	kJ/mol	Joback Method
hvap	87.05	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	5.296		Crippen Method
mcvol	307.660	ml/mol	McGowan Method
pc	1465.73	kPa	Joback Method
rinpol	2407.00		NIST Webbook
rinpol	2407.00		NIST Webbook
tb	897.52	K	Joback Method
tc	1114.32	K	Joback Method
tf	606.53	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	990.16	J/mol×K	897.52	Joback Method
cpg	1009.21	J/mol×K	933.65	Joback Method
cpg	1027.87	J/mol×K	969.79	Joback Method
cpg	1046.31	J/mol×K	1005.92	Joback Method
cpg	1064.69	J/mol×K	1042.05	Joback Method
cpg	1083.18	J/mol×K	1078.19	Joback Method
cpg	1101.94	J/mol×K	1114.32	Joback Method

Sources

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=C55285148&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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