Dioxacarb

Other names:	2-(1,3-Dioxolan-2-yl)phenyl methylcarbamate
	2-(1,3-Dioxolan-2-yl)phenyl-N-methylcarbamat
	2-(1,3-Dioxolane-2-yl)phenyl N-methylcarbamate
	C-8353
	CIBA 8353
	CIBA C 8353
	Carbamic acid, methyl-, o-(1,3-dioxolan-2-yl)phenyl ester
	DU PONT 1519
	Dioxacarbe
	Dioxocarb
	Du Pont insecticide 1519
	ENT 27,389
	Elecron 50
	Elocron
	Elocron 50WP
	Elocron 8353
	Famid
	MCDP
	NSC 190981
	Phenol, 2-(1,3-dioxolan-2-yl)-, methylcarbamate
	Rovlinka
	o-(1,3-Dioxolan-2-yl)phenyl methylcarbamate
Inchi:	InChI=1S/C11H13NO4/c1-12-11(13)16-9-5-3-2-4-8(9)10-14-6-7-15-10/h2-5,10H,6-7H2,1
InchiKey:	SDKQRNRRDYRQKY-UHFFFAOYSA-N
Formula:	C10H13NO4
SMILES:	CNC(=O)Oc1ccccc1C1OCCO1
Mol. weight [g/mol]:	211.21
CAS:	6988-21-2

Physical Properties

Property code	Value	Unit	Source
gf	-135.70	kJ/mol	Joback Method
hf	-440.16	kJ/mol	Joback Method
hfus	35.68	kJ/mol	Joback Method
hvap	67.89	kJ/mol	Joback Method
log10ws	-1.57		Aqueous Solubility Prediction Method

log10ws	-1.57		Estimated Solubility Method
logp	1.450		Crippen Method
mcvol	160.390	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
tb	678.38	K	Joback Method
tc	912.51	K	Joback Method
tf	388.27 ± 0.20	K	NIST Webbook
tf	387.65	K	Aqueous Solubility Prediction Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.15	J/mol×K	678.38	Joback Method
cpg	457.72	J/mol×K	717.40	Joback Method
cpg	471.18	J/mol×K	756.42	Joback Method
cpg	483.56	J/mol×K	795.45	Joback Method
cpg	494.89	J/mol×K	834.47	Joback Method
cpg	505.20	J/mol×K	873.49	Joback Method
cpg	514.53	J/mol×K	912.51	Joback Method
hfust	23.82	kJ/mol	387.20	NIST Webbook

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6988212&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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