

Hydracrylic acid, 2-(carboxyamino)-, dibenzyl ester, chloroacetate

Other names:	Serine, n-carboxy-, dibenzyl ester, chloroacetate (ester)
Inchi:	InChI=1S/C20H20ClNO6/c21-11-18(23)26-14-17(19(24)27-12-15-7-3-1-4-8-15)22-20(25)
InchiKey:	FFGNBQLGIGNAMP-UHFFFAOYSA-N
Formula:	C20H20ClNO6
SMILES:	O=C(CCl)OCC(N=C(O)OCc1ccccc1)C(=O)OCc1ccccc1
Mol. weight [g/mol]:	405.83
CAS:	6335-07-5

Physical Properties

Property code	Value	Unit	Source
hf	-705.71	kJ/mol	Joback Method
hvap	109.46	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.011		Crippen Method
mcvol	289.680	ml/mol	McGowan Method
pc	1682.41	kPa	Joback Method
tb	1091.09	K	Joback Method
tc	1337.45	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6335075&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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