DIETHOFENCARB

Other names: Isopropyl N-(3,4-diethoxyphenyl)carbamate
Carbamic acid, N-(3,4-diethoxyphenyl)-, 1-methylethyl ester
*
Inchi: InChI=1S/C14H21NO4/c1-5-17-12-8-7-11(9-13(12)18-6-2)15-14(16)19-10(3)4/h7-10H,5-
InchiKey: LNJNFVJKDJYTEU-UHFFFAOYSA-N
Formula: C14H21NO4
SMILES: CCOc1ccc(NC(=O)OC(C)C)cc1OCC
Mol. weight [g/mol]: 267.32
CAS: 87130-20-9

Physical Properties

Property code	Value	Unit	Source
gf	-196.82	kJ/mol	Joback Method
hf	-579.75	kJ/mol	Joback Method
hfus	32.02	kJ/mol	Joback Method
hvap	70.38	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.441		Crippen Method
mcvol	213.520	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	1993.00		NIST Webbook
rinpol	1993.00		NIST Webbook
rinpol	1979.00		NIST Webbook
rinpol	1979.00		NIST Webbook
tb	727.22	K	Joback Method
tc	929.92	K	Joback Method
tf	453.28	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.78	J/mol×K	727.22	Joback Method
cpg	618.92	J/mol×K	761.00	Joback Method

cpg	633.13	J/mol×K	794.79	Joback Method
cpg	646.39	J/mol×K	828.57	Joback Method
cpg	658.71	J/mol×K	862.35	Joback Method
cpg	670.07	J/mol×K	896.14	Joback Method
cpg	680.47	J/mol×K	929.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87130209&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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