

Dulcin (p-ethoxyphenyl carbamide) methylated

Inchi:	InChI=1S/C12H18N2O2/c1-5-16-11-8-6-10(7-9-11)14(4)12(15)13(2)3/h6-9H,5H2,1-4H3
InchiKey:	QSBJERBFVVXMCV-UHFFFAOYSA-N
Formula:	C12H18N2O2
SMILES:	CCOc1ccc(N(C)C(=O)N(C)C)cc1
Mol. weight [g/mol]:	222.28

Physical Properties

Property code	Value	Unit	Source
gf	140.58	kJ/mol	Joback Method
hf	-175.69	kJ/mol	Joback Method
hfus	29.32	kJ/mol	Joback Method
hvap	58.49	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	2.203		Crippen Method
mvol	183.580	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
rinpol	1310.00		NIST Webbook
tb	606.79	K	Joback Method
tc	808.35	K	Joback Method
tf	401.04	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.41	J/molxK	606.79	Joback Method
cpg	483.21	J/molxK	640.38	Joback Method
cpg	498.07	J/molxK	673.98	Joback Method
cpg	512.04	J/molxK	707.57	Joback Method
cpg	525.13	J/molxK	741.16	Joback Method
cpg	537.39	J/molxK	774.76	Joback Method
cpg	548.84	J/molxK	808.35	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=R524879&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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