iso-Butyl n-methyl anthranilate

Other names: iso-Butyl N-methyl anthranilate
isobutyl 2-(methylamino)benzoate
Inchi: InChI=1S/C12H17NO2/c1-9(2)8-15-12(14)10-6-4-5-7-11(10)13-3/h4-7,9,13H,8H2,1-3H3
InchiKey: WKYZGTHZBSYUFI-UHFFFAOYSA-N
Formula: C12H17NO2
SMILES: CNc1ccccc1C(=O)OCC(C)C
Mol. weight [g/mol]: 207.27

Physical Properties

Property code	Value	Unit	Source
hf	-350.31	kJ/mol	Cheméo Relay (1.0)
hfus	24.85	kJ/mol	Joback Method
hvap	72.63	kJ/mol	Cheméo Relay (1.0)
ie	7.70	eV	Cheméo Relay (1.0)
log10ws	-3.66		Cheméo Relay (1.0)
logp	2.541		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
rinpol	1617.00		NIST Webbook
ripol	2174.00		NIST Webbook
ripol	2174.00		NIST Webbook
tb	566.81	K	Cheméo Relay (1.0)
tf	294.11	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.86	J/mol×K	631.64	Joback Method
cpg	460.85	J/mol×K	666.80	Joback Method
cpg	474.96	J/mol×K	701.96	Joback Method
cpg	488.20	J/mol×K	737.13	Joback Method
cpg	500.60	J/mol×K	772.29	Joback Method
cpg	512.17	J/mol×K	807.45	Joback Method
cpg	522.93	J/mol×K	842.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65505240&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point