

Benzoic acid, 2-amino-, propyl ester

Other names:	propyl anthranilate propyl 2-aminobenzoate
Inchi:	InChI=1S/C10H13NO2/c1-2-7-13-10(12)8-5-3-4-6-9(8)11/h3-6H,2,7,11H2,1H3
InchiKey:	QYGHESHPPSSONP-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	CCCOC(=O)c1ccccc1N
Mol. weight [g/mol]:	179.22
CAS:	30954-98-4

Physical Properties

Property code	Value	Unit	Source
gf	-31.37	kJ/mol	Joback Method
hf	-235.68	kJ/mol	Joback Method
hfus	23.29	kJ/mol	Joback Method
hvap	60.59	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.836		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
rinpol	1500.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1500.00		NIST Webbook
ripol	2320.00		NIST Webbook
tb	608.68	K	Joback Method
tc	830.79	K	Joback Method
tf	396.82	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.09	J/molxK	608.68	Joback Method
cpg	370.13	J/molxK	645.70	Joback Method

cpg	382.38	J/mol×K	682.72	Joback Method
cpg	393.85	J/mol×K	719.74	Joback Method
cpg	404.56	J/mol×K	756.76	Joback Method
cpg	414.52	J/mol×K	793.78	Joback Method
cpg	423.76	J/mol×K	830.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30954984&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

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
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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