1-Butanol, 3-methyl-, 4-nitrobenzoate

Other names: 4-Nitrobenzoic acid, 3-methylbutyl ester
Benzoic acid, 4-nitro, 3-methylbutyl ester
isopentyl 4-nitrobenzoate
Inchi: InChI=1S/C12H15NO4/c1-9(2)7-8-17-12(14)10-3-5-11(6-4-10)13(15)16/h3-6,9H,7-8H2,1
InchiKey: KMOODDWVCAWHMC-UHFFFAOYSA-N
Formula: C12H15NO4
SMILES: CC(C)CCOC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 237.25
CAS: 38120-06-8

Physical Properties

Property code	Value	Unit	Source
gf	-47.87	kJ/mol	Joback Method
hf	-326.79	kJ/mol	Joback Method
hfus	31.11	kJ/mol	Joback Method
hvap	70.60	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	2.798		Crippen Method
mcvol	181.040	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	1765.00		NIST Webbook
rinpol	1759.00		NIST Webbook
rinpol	1759.00		NIST Webbook
rinpol	1764.00		NIST Webbook
rinpol	1781.00		NIST Webbook
ripol	2522.00		NIST Webbook
ripol	2526.00		NIST Webbook
ripol	2547.00		NIST Webbook
ripol	2567.00		NIST Webbook
tb	733.31	K	Joback Method
tc	966.01	K	Joback Method
tf	464.71	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.12	J/mol×K	733.31	Joback Method
cpg	511.61	J/mol×K	772.09	Joback Method
cpg	524.08	J/mol×K	810.88	Joback Method
cpg	535.55	J/mol×K	849.66	Joback Method
cpg	546.05	J/mol×K	888.45	Joback Method
cpg	555.62	J/mol×K	927.23	Joback Method
cpg	564.27	J/mol×K	966.01	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38120068&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume