butyl 3,5-dinitrobenzoate

Inchi: InChI=1S/C11H12N2O6/c1-2-3-4-19-11(14)8-5-9(12(15)16)7-10(6-8)13(17)18/h5-7H,2-4
InchiKey: LDMPZJOBKLVTKW-UHFFFAOYSA-N
Formula: C11H12N2O6
SMILES: CCCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 268.22
CAS: 10478-02-1

Physical Properties

Property code	Value	Unit	Source
gf	-27.93	kJ/mol	Joback Method
hf	-323.10	kJ/mol	Joback Method
hfus	43.02	kJ/mol	Joback Method
hvap	86.02	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	2.460		Crippen Method
mcvol	184.370	ml/mol	McGowan Method
pc	2761.36	kPa	Joback Method
rinpol	1957.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	1975.00		NIST Webbook
rinpol	1959.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1942.00		NIST Webbook
rinpol	1942.00		NIST Webbook
rinpol	1957.00		NIST Webbook
ripol	2873.00		NIST Webbook
ripol	2906.00		NIST Webbook
ripol	2906.00		NIST Webbook
ripol	2898.00		NIST Webbook
ripol	2873.00		NIST Webbook
ripol	2915.00		NIST Webbook
tb	867.69	K	Joback Method
tc	1118.15	K	Joback Method
tf	624.57	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.98	J/mol×K	867.69	Joback Method
cpg	544.03	J/mol×K	909.43	Joback Method
cpg	553.01	J/mol×K	951.18	Joback Method
cpg	560.96	J/mol×K	992.92	Joback Method
cpg	567.90	J/mol×K	1034.67	Joback Method
cpg	573.89	J/mol×K	1076.41	Joback Method
cpg	578.93	J/mol×K	1118.15	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10478021&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