3-Methylbutan-2-yl 3,5-dinitrobenzoate

Other names: Benzoic acid, 3,5-dinitro, 1,2-dimethylpropyl ester
Inchi: InChI=1S/C12H14N2O6/c1-7(2)8(3)20-12(15)9-4-10(13(16)17)6-11(5-9)14(18)19/h4-8H,
InchiKey: XOORMJSSSMWQQQ-UHFFFAOYSA-N
Formula: C12H14N2O6
SMILES: CC(C)C(C)OC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 282.25

Physical Properties

Property code	Value	Unit	Source
gf	-24.39	kJ/mol	Joback Method
hf	-354.30	kJ/mol	Joback Method
hfus	38.56	kJ/mol	Joback Method
hvap	87.47	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	2.704		Crippen Method
mcvol	198.460	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
rinpol	1940.00		NIST Webbook
rinpol	1955.00		NIST Webbook
rinpol	1933.00		NIST Webbook
rinpol	1933.00		NIST Webbook
rinpol	1953.00		NIST Webbook
ripol	2806.00		NIST Webbook
ripol	2790.00		NIST Webbook
ripol	2805.00		NIST Webbook
ripol	2827.00		NIST Webbook
tb	889.69	K	Joback Method
tc	1143.97	K	Joback Method
tf	605.84	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	589.74	J/mol×K	889.69	Joback Method
cpg	600.34	J/mol×K	932.07	Joback Method
cpg	609.75	J/mol×K	974.45	Joback Method
cpg	618.02	J/mol×K	1016.83	Joback Method
cpg	625.17	J/mol×K	1059.21	Joback Method
cpg	631.25	J/mol×K	1101.59	Joback Method
cpg	636.29	J/mol×K	1143.97	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373863&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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