octyl 3,5-dinitrobenzoate

Other names: Benzoic acid, 3,5-dinitro, octyl ester
Inchi: InChI=1S/C15H20N2O6/c1-2-3-4-5-6-7-8-23-15(18)12-9-13(16(19)20)11-14(10-12)17(21
InchiKey: UUJMMZMVYHKYGJ-UHFFFAOYSA-N
Formula: C15H20N2O6
SMILES: CCCCCCCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 324.33
CAS: 10478-06-5

Physical Properties

Property code	Value	Unit	Source
gf	5.75	kJ/mol	Joback Method
hf	-405.66	kJ/mol	Joback Method
hfus	53.38	kJ/mol	Joback Method
hvap	94.92	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	4.020		Crippen Method
mcvol	240.730	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	2343.00		NIST Webbook
rinpol	2343.00		NIST Webbook
rinpol	2355.00		NIST Webbook
rinpol	2368.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2343.00		NIST Webbook
rinpol	2370.00		NIST Webbook
rinpol	2370.00		NIST Webbook
ripol	3265.00		NIST Webbook
ripol	3288.00		NIST Webbook
ripol	3305.00		NIST Webbook
ripol	3313.00		NIST Webbook
ripol	3313.00		NIST Webbook
ripol	3265.00		NIST Webbook
ripol	3265.00		NIST Webbook
tb	959.21	K	Joback Method
tc	1197.77	K	Joback Method
tf	669.65	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.28	J/mol×K	959.21	Joback Method
cpg	768.30	J/mol×K	998.97	Joback Method
cpg	778.18	J/mol×K	1038.73	Joback Method
cpg	786.96	J/mol×K	1078.49	Joback Method
cpg	794.69	J/mol×K	1118.25	Joback Method
cpg	801.42	J/mol×K	1158.01	Joback Method
cpg	807.19	J/mol×K	1197.77	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=C10478065&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