heptyl 3,5-dinitrobenzoate

Other names: Benzoic acid, 3,5-dinitro, heptyl ester
Inchi: InChI=1S/C14H18N2O6/c1-2-3-4-5-6-7-22-14(17)11-8-12(15(18)19)10-13(9-11)16(20)21
InchiKey: SALJFNLCUUKOMX-UHFFFAOYSA-N
Formula: C14H18N2O6
SMILES: CCCCCCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 310.30

Physical Properties

Property code	Value	Unit	Source
gf	-2.67	kJ/mol	Joback Method
hf	-385.02	kJ/mol	Joback Method
hfus	50.79	kJ/mol	Joback Method
hvap	92.70	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	3.630		Crippen Method
mcvol	226.640	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	2236.00		NIST Webbook
rinpol	2269.00		NIST Webbook
rinpol	2256.00		NIST Webbook
rinpol	2244.00		NIST Webbook
rinpol	2281.00		NIST Webbook
rinpol	2266.00		NIST Webbook
rinpol	2244.00		NIST Webbook
rinpol	2244.00		NIST Webbook
rinpol	2281.00		NIST Webbook
ripol	3164.00		NIST Webbook
ripol	3210.00		NIST Webbook
ripol	3205.00		NIST Webbook
ripol	3189.00		NIST Webbook
ripol	3164.00		NIST Webbook
ripol	3164.00		NIST Webbook
ripol	3210.00		NIST Webbook
tb	936.33	K	Joback Method
tc	1176.75	K	Joback Method
tf	658.38	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.28	J/mol×K	936.33	Joback Method
cpg	711.12	J/mol×K	976.40	Joback Method
cpg	720.84	J/mol×K	1016.47	Joback Method
cpg	729.47	J/mol×K	1056.54	Joback Method
cpg	737.07	J/mol×K	1096.61	Joback Method
cpg	743.67	J/mol×K	1136.68	Joback Method
cpg	749.32	J/mol×K	1176.75	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=R35086&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