Acetic acid, (3-methyl-2-nitrophenyl)methyl ester

Inchi: InChI=1S/C10H11NO4/c1-7-4-3-5-9(6-15-8(2)12)10(7)11(13)14/h3-5H,6H2,1-2H3
InchiKey: QVXJMKNZIUTYBV-UHFFFAOYSA-N
Formula: C10H11NO4
SMILES: CC(=O)OCc1cccc(C)c1[N+](=O)[O-]
Mol. weight [g/mol]: 209.20

Physical Properties

Property code	Value	Unit	Source
gf	-71.90	kJ/mol	Joback Method
hf	-291.70	kJ/mol	Joback Method
hfus	29.07	kJ/mol	Joback Method
hvap	67.20	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	1.966		Crippen Method
mcvol	152.860	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	1581.00		NIST Webbook
tb	692.97	K	Joback Method
tc	931.12	K	Joback Method
tf	469.69	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.70	J/mol×K	692.97	Joback Method
cpg	405.71	J/mol×K	732.66	Joback Method
cpg	416.84	J/mol×K	772.35	Joback Method
cpg	427.10	J/mol×K	812.05	Joback Method
cpg	436.50	J/mol×K	851.74	Joback Method
cpg	445.08	J/mol×K	891.43	Joback Method
cpg	452.83	J/mol×K	931.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368210&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume