3-Buten-2-one, 3-nitro-4-phenyl-, (E)-

Inchi: InChI=1S/C10H9NO3/c1-8(12)10(11(13)14)7-9-5-3-2-4-6-9/h2-7H,1H3/b10-7-
InchiKey: OYRPMZZLRMIPOM-YFHOEESVSA-N
Formula: C10H9NO3
SMILES: CC(=O)C(=Cc1ccccc1)[N+](=O)[O-]
Mol. weight [g/mol]: 191.18
CAS: 58321-86-1

Physical Properties

Property code	Value	Unit	Source
gf	124.03	kJ/mol	Joback Method
hf	-29.11	kJ/mol	Joback Method
hfus	27.55	kJ/mol	Joback Method
hvap	63.50	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	1.893		Crippen Method
mcvol	142.690	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
tb	664.63	K	Joback Method
tc	919.67	K	Joback Method
tf	403.38	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.78	J/mol×K	664.63	Joback Method
cpg	361.80	J/mol×K	707.14	Joback Method
cpg	372.77	J/mol×K	749.64	Joback Method
cpg	382.80	J/mol×K	792.15	Joback Method
cpg	391.97	J/mol×K	834.66	Joback Method
cpg	400.36	J/mol×K	877.17	Joback Method
cpg	408.08	J/mol×K	919.67	Joback Method

Sources

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=C58321861&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:
https://www.chemeo.com/cid/18-665-4/3-Buten-2-one-3-nitro-4-phenyl-E.pdf
Generated by Cheméo on 2024-04-23 16:37:25.306825201 +0000 UTC m=+16179494.227402516.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.