Benzeneacetic acid, nonyl ester

Other names: Phenylacetic acid, nonyl ester
nonyl phenylacetate
Inchi: InChI=1S/C17H26O2/c1-2-3-4-5-6-7-11-14-19-17(18)15-16-12-9-8-10-13-16/h8-10,12-13
InchiKey: QICYMLLAPDCBNZ-UHFFFAOYSA-N
Formula: C17H26O2
SMILES: CCCCCCCCCOC(=O)Cc1ccccc1
Mol. weight [g/mol]: 262.39
CAS: 72109-82-1

Physical Properties

Property code	Value	Unit	Source
gf	-29.25	kJ/mol	Joback Method
hf	-402.48	kJ/mol	Joback Method
hfus	36.61	kJ/mol	Joback Method
hvap	64.87	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.523		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1635.13	kPa	Joback Method
rinpol	1906.65		NIST Webbook
rinpol	1935.31		NIST Webbook
tb	691.33	K	Joback Method
tc	884.75	K	Joback Method
tf	379.93	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.86	J/mol×K	691.33	Joback Method
cpg	732.85	J/mol×K	852.51	Joback Method
cpg	719.09	J/mol×K	820.27	Joback Method
cpg	704.44	J/mol×K	788.04	Joback Method
cpg	688.87	J/mol×K	755.80	Joback Method

cpg	672.36	J/mol×K	723.57	Joback Method
cpg	745.76	J/mol×K	884.75	Joback Method
dvisc	0.0001083	Pa×s	691.33	Joback Method
dvisc	0.0001421	Pa×s	639.43	Joback Method
dvisc	0.0001956	Pa×s	587.53	Joback Method
dvisc	0.0002864	Pa×s	535.63	Joback Method
dvisc	0.0004552	Pa×s	483.73	Joback Method
dvisc	0.0008086	Pa×s	431.83	Joback Method
dvisc	0.0016807	Pa×s	379.93	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C72109821&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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