Butanoic acid, nonyl ester

Other names: Nonyl butyrate
Inchi: InChI=1S/C13H26O2/c1-3-5-6-7-8-9-10-12-15-13(14)11-4-2/h3-12H2,1-2H3
InchiKey: RVNCBAPCNVAWOY-UHFFFAOYSA-N
Formula: C13H26O2
SMILES: CCCCCCCCCOC(=O)CCC
Mol. weight [g/mol]: 214.34
CAS: 2639-64-7

Physical Properties

Property code	Value	Unit	Source
gf	-175.34	kJ/mol	Joback Method
hf	-556.45	kJ/mol	Joback Method
hfus	32.21	kJ/mol	Joback Method
hvap	53.69	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.080		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
rinpol	1461.00		NIST Webbook
rinpol	1466.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1489.00		NIST Webbook
ripol	1724.00		NIST Webbook
ripol	1728.00		NIST Webbook
tb	535.00 ± 6.00	K	NIST Webbook
tc	741.92	K	Joback Method
tf	308.43	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.80	J/mol×K	573.13	Joback Method
cpg	531.11	J/mol×K	601.26	Joback Method
cpg	546.77	J/mol×K	629.39	Joback Method
cpg	561.79	J/mol×K	657.52	Joback Method
cpg	576.19	J/mol×K	685.66	Joback Method
cpg	589.97	J/mol×K	713.79	Joback Method
cpg	603.14	J/mol×K	741.92	Joback Method
dvisc	0.0029408	Pa×s	308.43	Joback Method
dvisc	0.0013589	Pa×s	352.55	Joback Method
dvisc	0.0007456	Pa×s	396.66	Joback Method
dvisc	0.0004613	Pa×s	440.78	Joback Method
dvisc	0.0003115	Pa×s	484.90	Joback Method
dvisc	0.0002245	Pa×s	529.01	Joback Method
dvisc	0.0001702	Pa×s	573.13	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=C2639647&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume