Butanedioic acid, nonyl phenylmethyl ester

Other names: Nonyl benzyl succinate
Inchi: InChI=1S/C20H30O4/c1-2-3-4-5-6-7-11-16-23-19(21)14-15-20(22)24-17-18-12-9-8-10-13
InchiKey: LZXXTGLTBYLDBX-UHFFFAOYSA-N
Formula: C20H30O4
SMILES: CCCCCCCCCOC(=O)CCC(=O)OCc1ccccc1
Mol. weight [g/mol]: 334.45
CAS: 119450-17-8

Physical Properties

Property code	Value	Unit	Source
gf	-237.91	kJ/mol	Joback Method
hf	-709.20	kJ/mol	Joback Method
hfus	47.17	kJ/mol	Joback Method
hvap	80.70	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.804		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1356.63	kPa	Joback Method
rinpol	2448.00		NIST Webbook
rinpol	2448.00		NIST Webbook
tb	836.26	K	Joback Method
tc	1035.40	K	Joback Method
tf	485.90	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.33	J/mol×K	836.26	Joback Method
cpg	894.55	J/mol×K	869.45	Joback Method
cpg	909.64	J/mol×K	902.64	Joback Method
cpg	923.63	J/mol×K	935.83	Joback Method
cpg	936.55	J/mol×K	969.02	Joback Method
cpg	948.42	J/mol×K	1002.21	Joback Method

cpg	959.28	J/mol×K	1035.40	Joback Method
dvisc	0.0006973	Pa×s	485.90	Joback Method
dvisc	0.0003625	Pa×s	544.29	Joback Method
dvisc	0.0002139	Pa×s	602.69	Joback Method
dvisc	0.0001385	Pa×s	661.08	Joback Method
dvisc	0.0000963	Pa×s	719.47	Joback Method
dvisc	0.0000707	Pa×s	777.87	Joback Method
dvisc	0.0000542	Pa×s	836.26	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C119450178&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.