Butanedioic acid, pentyl phenylmethyl ester

Other names: Pentyl benzyl succinate
Inchi: InChI=1S/C16H22O4/c1-2-3-7-12-19-15(17)10-11-16(18)20-13-14-8-5-4-6-9-14/h4-6,8-9
InchiKey: GVUYTZKKCMNYGB-UHFFFAOYSA-N
Formula: C16H22O4
SMILES: CCCCCOC(=O)CCC(=O)OCc1ccccc1
Mol. weight [g/mol]: 278.34
CAS: 119450-13-4

Physical Properties

Property code	Value	Unit	Source
gf	-271.59	kJ/mol	Joback Method
hf	-626.64	kJ/mol	Joback Method
hfus	36.81	kJ/mol	Joback Method
hvap	71.80	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.243		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	2045.00		NIST Webbook
tb	744.74	K	Joback Method
tc	945.71	K	Joback Method
tf	440.82	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.23	J/mol×K	744.74	Joback Method
cpg	664.46	J/mol×K	778.23	Joback Method
cpg	678.71	J/mol×K	811.73	Joback Method
cpg	691.99	J/mol×K	845.22	Joback Method
cpg	704.32	J/mol×K	878.72	Joback Method
cpg	715.72	J/mol×K	912.21	Joback Method
cpg	726.20	J/mol×K	945.71	Joback Method

dvisc	0.0010214	Pa×s	440.82	Joback Method
dvisc	0.0005579	Pa×s	491.47	Joback Method
dvisc	0.0003411	Pa×s	542.13	Joback Method
dvisc	0.0002269	Pa×s	592.78	Joback Method
dvisc	0.0001609	Pa×s	643.43	Joback Method
dvisc	0.0001200	Pa×s	694.09	Joback Method
dvisc	0.0000931	Pa×s	744.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119450134&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
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