Butanedioic acid, butyl phenylmethyl ester

Other names: Butyl benzyl succinate
Succinic acid, benzyl butyl ester
Inchi: InChI=1S/C15H20O4/c1-2-3-11-18-14(16)9-10-15(17)19-12-13-7-5-4-6-8-13/h4-8H,2-3,9
InchiKey: SISDVYCKRJTJHA-UHFFFAOYSA-N
Formula: C15H20O4
SMILES: CCCCOC(=O)CCC(=O)OCc1ccccc1
Mol. weight [g/mol]: 264.32
CAS: 1223-37-6

Physical Properties

Property code	Value	Unit	Source
gf	-280.01	kJ/mol	Joback Method
hf	-606.00	kJ/mol	Joback Method
hfus	34.22	kJ/mol	Joback Method
hvap	69.57	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.853		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	1941.00		NIST Webbook
tb	721.86	K	Joback Method
tc	924.67	K	Joback Method
tf	429.55	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.46	J/mol×K	721.86	Joback Method
cpg	609.36	J/mol×K	755.66	Joback Method
cpg	623.31	J/mol×K	789.46	Joback Method
cpg	636.32	J/mol×K	823.26	Joback Method
cpg	648.41	J/mol×K	857.07	Joback Method
cpg	659.60	J/mol×K	890.87	Joback Method

cpg	669.89	J/mol×K	924.67	Joback Method
dvisc	0.0011088	Pa×s	429.55	Joback Method
dvisc	0.0006139	Pa×s	478.27	Joback Method
dvisc	0.0003792	Pa×s	526.99	Joback Method
dvisc	0.0002541	Pa×s	575.70	Joback Method
dvisc	0.0001812	Pa×s	624.42	Joback Method
dvisc	0.0001358	Pa×s	673.14	Joback Method
dvisc	0.0001057	Pa×s	721.86	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=C1223376&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

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