Butanedioic acid, phenylmethyl propyl ester

Other names: Propyl benzyl succinate
Inchi: InChI=1S/C14H18O4/c1-2-10-17-13(15)8-9-14(16)18-11-12-6-4-3-5-7-12/h3-7H,2,8-11H
InchiKey: LQITZYVBKYLNJM-UHFFFAOYSA-N
Formula: C14H18O4
SMILES: CCCOC(=O)CCC(=O)OCc1ccccc1
Mol. weight [g/mol]: 250.29
CAS: 119450-12-3

Physical Properties

Property code	Value	Unit	Source
gf	-288.43	kJ/mol	Joback Method
hf	-585.36	kJ/mol	Joback Method
hfus	31.63	kJ/mol	Joback Method
hvap	67.35	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.463		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	1842.00		NIST Webbook
rinpol	1842.00		NIST Webbook
tb	698.98	K	Joback Method
tc	904.10	K	Joback Method
tf	418.28	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.84	J/mol×K	698.98	Joback Method
cpg	604.37	J/mol×K	869.91	Joback Method
cpg	593.45	J/mol×K	835.72	Joback Method
cpg	581.65	J/mol×K	801.54	Joback Method
cpg	568.96	J/mol×K	767.35	Joback Method
cpg	555.36	J/mol×K	733.17	Joback Method

cpg	614.42	J/mol×K	904.10	Joback Method
dvisc	0.0001196	Pa×s	698.98	Joback Method
dvisc	0.0001529	Pa×s	652.20	Joback Method
dvisc	0.0002032	Pa×s	605.41	Joback Method
dvisc	0.0002831	Pa×s	558.63	Joback Method
dvisc	0.0004192	Pa×s	511.85	Joback Method
dvisc	0.0006717	Pa×s	465.06	Joback Method
dvisc	0.0011960	Pa×s	418.28	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=C119450123&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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