Butanedioic acid, hexyl phenylmethyl ester

Other names: Hexyl benzyl succinate
Inchi: InChI=1S/C17H24O4/c1-2-3-4-8-13-20-16(18)11-12-17(19)21-14-15-9-6-5-7-10-15/h5-7,
InchiKey: IROBBPAWTAUBOK-UHFFFAOYSA-N
Formula: C17H24O4
SMILES: CCCCCCOC(=O)CCC(=O)OCc1ccccc1
Mol. weight [g/mol]: 292.37
CAS: 119450-14-5

Physical Properties

Property code	Value	Unit	Source
gf	-263.17	kJ/mol	Joback Method
hf	-647.28	kJ/mol	Joback Method
hfus	39.40	kJ/mol	Joback Method
hvap	74.02	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.633		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	2143.00		NIST Webbook
rinpol	2143.00		NIST Webbook
tb	767.62	K	Joback Method
tc	967.25	K	Joback Method
tf	452.09	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.09	J/mol×K	767.62	Joback Method
cpg	720.60	J/mol×K	800.89	Joback Method
cpg	735.10	J/mol×K	834.16	Joback Method
cpg	748.60	J/mol×K	867.43	Joback Method
cpg	761.13	J/mol×K	900.71	Joback Method
cpg	772.69	J/mol×K	933.98	Joback Method

cpg	783.32	J/mol×K	967.25	Joback Method
dvisc	0.0009355	Pa×s	452.09	Joback Method
dvisc	0.0005043	Pa×s	504.68	Joback Method
dvisc	0.0003054	Pa×s	557.27	Joback Method
dvisc	0.0002017	Pa×s	609.86	Joback Method
dvisc	0.0001423	Pa×s	662.44	Joback Method
dvisc	0.0001057	Pa×s	715.03	Joback Method
dvisc	0.0000817	Pa×s	767.62	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=C119450145&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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