Butanedioic acid, ethyl phenylmethyl ester

Other names: Ethyl benzyl succinate
Inchi: InChI=1S/C13H16O4/c1-2-16-12(14)8-9-13(15)17-10-11-6-4-3-5-7-11/h3-7H,2,8-10H2,1
InchiKey: MGWTXNMQOXXVRU-UHFFFAOYSA-N
Formula: C13H16O4
SMILES: CCOC(=O)CCC(=O)OCc1ccccc1
Mol. weight [g/mol]: 236.26
CAS: 106478-00-6

Physical Properties

Property code	Value	Unit	Source
gf	-296.85	kJ/mol	Joback Method
hf	-564.72	kJ/mol	Joback Method
hfus	29.04	kJ/mol	Joback Method
hvap	65.12	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.073		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinpol	1740.00		NIST Webbook
tb	676.10	K	Joback Method
tc	883.94	K	Joback Method
tf	407.01	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.48	J/mol×K	676.10	Joback Method
cpg	550.07	J/mol×K	849.30	Joback Method
cpg	539.47	J/mol×K	814.66	Joback Method
cpg	528.02	J/mol×K	780.02	Joback Method
cpg	515.71	J/mol×K	745.38	Joback Method
cpg	502.54	J/mol×K	710.74	Joback Method
cpg	559.82	J/mol×K	883.94	Joback Method

dvisc	0.0001346	Pa×s	676.10	Joback Method
dvisc	0.0001714	Pa×s	631.25	Joback Method
dvisc	0.0002266	Pa×s	586.40	Joback Method
dvisc	0.0003138	Pa×s	541.56	Joback Method
dvisc	0.0004608	Pa×s	496.71	Joback Method
dvisc	0.0007303	Pa×s	451.86	Joback Method
dvisc	0.0012811	Pa×s	407.01	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=C106478006&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