Butanedioic acid, heptyl phenylmethyl ester

Other names: Heptyl benzyl succinate
Inchi: InChI=1S/C18H26O4/c1-2-3-4-5-9-14-21-17(19)12-13-18(20)22-15-16-10-7-6-8-11-16/h6
InchiKey: FUJUROXWLMHXBQ-UHFFFAOYSA-N
Formula: C18H26O4
SMILES: CCCCCCCOC(=O)CCC(=O)OCc1ccccc1
Mol. weight [g/mol]: 306.40
CAS: 119450-15-6

Physical Properties

Property code	Value	Unit	Source
gf	-254.75	kJ/mol	Joback Method
hf	-667.92	kJ/mol	Joback Method
hfus	41.99	kJ/mol	Joback Method
hvap	76.25	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.024		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	2246.00		NIST Webbook
tb	790.50	K	Joback Method
tc	989.35	K	Joback Method
tf	463.36	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.94	J/mol×K	790.50	Joback Method
cpg	830.49	J/mol×K	956.21	Joback Method
cpg	818.79	J/mol×K	923.07	Joback Method
cpg	806.11	J/mol×K	889.92	Joback Method
cpg	792.42	J/mol×K	856.78	Joback Method
cpg	777.71	J/mol×K	823.64	Joback Method
cpg	841.23	J/mol×K	989.35	Joback Method

dvisc	0.0000715	Pa×s	790.50	Joback Method
dvisc	0.0000927	Pa×s	735.98	Joback Method
dvisc	0.0001253	Pa×s	681.45	Joback Method
dvisc	0.0001786	Pa×s	626.93	Joback Method
dvisc	0.0002723	Pa×s	572.41	Joback Method
dvisc	0.0004537	Pa×s	517.88	Joback Method
dvisc	0.0008523	Pa×s	463.36	Joback Method

Sources

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=C119450156&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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