

Succinic acid, 3-bromophenethyl propyl ester

Inchi: InChI=1S/C15H19BrO4/c1-2-9-19-14(17)6-7-15(18)20-10-8-12-4-3-5-13(16)11-12/h3-5,1
InchiKey: DMPTUAZUIRLFCN-UHFFFAOYSA-N
Formula: C15H19BrO4
SMILES: CCCOC(=O)CCC(=O)OCCc1cccc(Br)c1
Mol. weight [g/mol]: 343.21

Physical Properties

Property code	Value	Unit	Source
gf	-275.32	kJ/mol	Joback Method
hf	-591.14	kJ/mol	Joback Method
hfus	39.12	kJ/mol	Joback Method
hvap	76.67	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.268		Crippen Method
mvol	230.830	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
rinpol	2239.00		NIST Webbook
rinpol	2239.00		NIST Webbook
tb	793.00	K	Joback Method
tc	1006.77	K	Joback Method
tf	501.87	K	Joback Method
vc	0.877	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.16	J/molxK	793.00	Joback Method
cpg	688.74	J/molxK	971.14	Joback Method
cpg	679.29	J/molxK	935.51	Joback Method
cpg	668.93	J/molxK	899.88	Joback Method
cpg	657.63	J/molxK	864.26	Joback Method
cpg	645.38	J/molxK	828.63	Joback Method
cpg	697.29	J/molxK	1006.77	Joback Method
dvisc	0.0000885	Paxs	793.00	Joback Method

dvisc	0.0001107	Paxs	744.48	Joback Method
dvisc	0.0001429	Paxs	695.96	Joback Method
dvisc	0.0001917	Paxs	647.43	Joback Method
dvisc	0.0002696	Paxs	598.91	Joback Method
dvisc	0.0004028	Paxs	550.39	Joback Method
dvisc	0.0006502	Paxs	501.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381279&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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