

Succinic acid, 4-bromobenzyl isobutyl ester

Inchi:	InChI=1S/C15H19BrO4/c1-11(2)9-19-14(17)7-8-15(18)20-10-12-3-5-13(16)6-4-12/h3-6,1
InchiKey:	COSQZGDNYBGLCG-UHFFFAOYSA-N
Formula:	C15H19BrO4
SMILES:	CC(C)COC(=O)CCC(=O)OCc1ccc(Br)cc1
Mol. weight [g/mol]:	343.21

Physical Properties

Property code	Value	Unit	Source
gf	-277.76	kJ/mol	Joback Method
hf	-596.42	kJ/mol	Joback Method
hfus	35.59	kJ/mol	Joback Method
hvap	76.28	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.472		Crippen Method
mvol	230.830	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	2194.00		NIST Webbook
rinpol	2194.00		NIST Webbook
tb	792.56	K	Joback Method
tc	1009.47	K	Joback Method
tf	486.87	K	Joback Method
vc	0.872	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.74	J/molxK	792.56	Joback Method
cpg	646.15	J/molxK	828.71	Joback Method
cpg	658.55	J/molxK	864.86	Joback Method
cpg	669.96	J/molxK	901.02	Joback Method
cpg	680.39	J/molxK	937.17	Joback Method
cpg	689.87	J/molxK	973.32	Joback Method
cpg	698.43	J/molxK	1009.47	Joback Method
dvisc	0.0007265	Paxs	486.87	Joback Method

dvisc	0.0004243	Paxs	537.82	Joback Method
dvisc	0.0002720	Paxs	588.77	Joback Method
dvisc	0.0001871	Paxs	639.71	Joback Method
dvisc	0.0001361	Paxs	690.66	Joback Method
dvisc	0.0001033	Paxs	741.61	Joback Method
dvisc	0.0000813	Paxs	792.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382427&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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