

Succinic acid, 2-bromobenzyl ethyl ester

Inchi:	InChI=1S/C13H15BrO4/c1-2-17-12(15)7-8-13(16)18-9-10-5-3-4-6-11(10)14/h3-6H,2,7-9H
InchiKey:	XHMSQXMRFWRHLU-UHFFFAOYSA-N
Formula:	C13H15BrO4
SMILES:	CCOC(=O)CCC(=O)OCc1ccccc1Br
Mol. weight [g/mol]:	315.16

Physical Properties

Property code	Value	Unit	Source
gf	-292.16	kJ/mol	Joback Method
hf	-549.86	kJ/mol	Joback Method
hfus	33.94	kJ/mol	Joback Method
hvap	72.22	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	2.836		Crippen Method
mcvol	202.650	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	2020.00		NIST Webbook
rinpol	2020.00		NIST Webbook
tb	747.24	K	Joback Method
tc	966.26	K	Joback Method
tf	479.33	K	Joback Method
vc	0.765	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.38	J/molxK	747.24	Joback Method
cpg	536.84	J/molxK	783.74	Joback Method
cpg	548.40	J/molxK	820.25	Joback Method
cpg	559.06	J/molxK	856.75	Joback Method
cpg	568.84	J/molxK	893.25	Joback Method
cpg	577.76	J/molxK	929.75	Joback Method
cpg	585.84	J/molxK	966.26	Joback Method
dvisc	0.0007747	Paxs	479.33	Joback Method

dvisc	0.0004934	Paxs	523.98	Joback Method
dvisc	0.0003373	Paxs	568.63	Joback Method
dvisc	0.0002437	Paxs	613.29	Joback Method
dvisc	0.0001840	Paxs	657.94	Joback Method
dvisc	0.0001440	Paxs	702.59	Joback Method
dvisc	0.0001161	Paxs	747.24	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=U381115&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

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