

Succinic acid, 3-bromophenethyl hexyl ester

Inchi:	InChI=1S/C18H25BrO4/c1-2-3-4-5-12-22-17(20)9-10-18(21)23-13-11-15-7-6-8-16(19)14
InchiKey:	YIAPWNOMRYBGKM-UHFFFAOYSA-N
Formula:	C18H25BrO4
SMILES:	CCCCCOC(=O)CCC(=O)OCCc1cccc(Br)c1
Mol. weight [g/mol]:	385.29

Physical Properties

Property code	Value	Unit	Source
gf	-250.06	kJ/mol	Joback Method
hf	-653.06	kJ/mol	Joback Method
hfus	46.89	kJ/mol	Joback Method
hvap	83.35	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.439		Crippen Method
mvol	273.100	ml/mol	McGowan Method
pc	1640.43	kPa	Joback Method
rinpol	2533.00		NIST Webbook
rinpol	2533.00		NIST Webbook
tb	861.64	K	Joback Method
tc	1071.94	K	Joback Method
tf	535.68	K	Joback Method
vc	1.046	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.28	J/molxK	861.64	Joback Method
cpg	815.30	J/molxK	896.69	Joback Method
cpg	828.25	J/molxK	931.74	Joback Method
cpg	840.16	J/molxK	966.79	Joback Method
cpg	851.06	J/molxK	1001.84	Joback Method
cpg	860.97	J/molxK	1036.89	Joback Method
cpg	869.92	J/molxK	1071.94	Joback Method
dvisc	0.0004832	Paxs	535.68	Joback Method

dvisc	0.0002881	Paxs	590.01	Joback Method
dvisc	0.0001874	Paxs	644.33	Joback Method
dvisc	0.0001303	Paxs	698.66	Joback Method
dvisc	0.0000955	Paxs	752.99	Joback Method
dvisc	0.0000730	Paxs	807.31	Joback Method
dvisc	0.0000577	Paxs	861.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381284&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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