

Succinic acid, 4-bromophenethyl heptyl ester

Inchi: InChI=1S/C19H27BrO4/c1-2-3-4-5-6-14-23-18(21)11-12-19(22)24-15-13-16-7-9-17(20)1
InchiKey: MFPJNMGIHURHGU-UHFFFAOYSA-N
Formula: C19H27BrO4
SMILES: CCCCCCOC(=O)CCC(=O)OCCc1ccc(Br)cc1
Mol. weight [g/mol]: 399.32

Physical Properties

Property code	Value	Unit	Source
gf	-241.64	kJ/mol	Joback Method
hf	-673.70	kJ/mol	Joback Method
hfus	49.48	kJ/mol	Joback Method
hvap	85.57	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.829		Crippen Method
mcvol	287.190	ml/mol	McGowan Method
pc	1519.94	kPa	Joback Method
rinpol	2652.00		NIST Webbook
rinpol	2652.00		NIST Webbook
tb	884.52	K	Joback Method
tc	1095.03	K	Joback Method
tf	546.95	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.35	J/molxK	884.52	Joback Method
cpg	873.59	J/molxK	919.60	Joback Method
cpg	886.72	J/molxK	954.69	Joback Method
cpg	898.78	J/molxK	989.77	Joback Method
cpg	909.80	J/molxK	1024.86	Joback Method
cpg	919.80	J/molxK	1059.94	Joback Method
cpg	928.82	J/molxK	1095.03	Joback Method
dvisc	0.0004342	Paxs	546.95	Joback Method

dvisc	0.0002558	Paxs	603.21	Joback Method
dvisc	0.0001649	Paxs	659.47	Joback Method
dvisc	0.0001139	Paxs	715.73	Joback Method
dvisc	0.0000831	Paxs	772.00	Joback Method
dvisc	0.0000632	Paxs	828.26	Joback Method
dvisc	0.0000498	Paxs	884.52	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=U381437&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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