Succinic acid, di(7-bromoheptyl) ester

Inchi: InChI=1S/C18H32Br2O4/c19-13-7-3-1-5-9-15-23-17(21)11-12-18(22)24-16-10-6-2-4-8-14
InchiKey: XZGSZXXVINANJD-UHFFFAOYSA-N
Formula: C18H32Br2O4
SMILES: O=C(CCC(=O)OCCCCCCCBr)OCCCCCCCBr
Mol. weight [g/mol]: 472.25

Physical Properties

Property code	Value	Unit	Source
gf	-338.52	kJ/mol	Joback Method
hf	-851.79	kJ/mol	Joback Method
hfus	58.52	kJ/mol	Joback Method
hvap	86.84	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.544		Crippen Method
mcvol	314.360	ml/mol	McGowan Method
pc	1355.63	kPa	Joback Method
rinpol	2896.00		NIST Webbook
rinpol	2896.00		NIST Webbook
tb	896.14	K	Joback Method
tc	1099.72	K	Joback Method
tf	556.54	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	939.11	J/mol×K	896.14	Joback Method
cpg	953.87	J/mol×K	930.07	Joback Method
cpg	967.62	J/mol×K	964.00	Joback Method
cpg	980.40	J/mol×K	997.93	Joback Method
cpg	992.23	J/mol×K	1031.86	Joback Method
cpg	1003.15	J/mol×K	1065.79	Joback Method
cpg	1013.20	J/mol×K	1099.72	Joback Method
dvisc	0.0003990	Pa×s	556.54	Joback Method

dvisc	0.0002304	Pa×s	613.14	Joback Method
dvisc	0.0001460	Pa×s	669.74	Joback Method
dvisc	0.0000993	Pa×s	726.34	Joback Method
dvisc	0.0000714	Pa×s	782.94	Joback Method
dvisc	0.0000537	Pa×s	839.54	Joback Method
dvisc	0.0000419	Pa×s	896.14	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=U382408&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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