Succinic acid, di(8-bromooctyl) ester

Inchi: InChI=1S/C20H36Br2O4/c21-15-9-5-1-3-7-11-17-25-19(23)13-14-20(24)26-18-12-8-4-2-6-10-16-22
InchiKey: DLIYZUZTKOQDLX-UHFFFAOYSA-N
Formula: C20H36Br2O4
SMILES: O=C(CCC(=O)OCCCCCCCCCBr)OCCCCCCCCCBr
Mol. weight [g/mol]: 500.31

Physical Properties

Property code	Value	Unit	Source
gf	-321.68	kJ/mol	Joback Method
hf	-893.07	kJ/mol	Joback Method
hfus	63.70	kJ/mol	Joback Method
hvap	91.30	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	6.324		Crippen Method
mcvol	342.540	ml/mol	McGowan Method
pc	1182.53	kPa	Joback Method
rinpol	3190.00		NIST Webbook
rinpol	3190.00		NIST Webbook
tb	941.90	K	Joback Method
tc	1153.20	K	Joback Method
tf	579.08	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1059.29	J/mol×K	941.90	Joback Method
cpg	1126.13	J/mol×K	1117.99	Joback Method
cpg	1114.85	J/mol×K	1082.77	Joback Method
cpg	1102.58	J/mol×K	1047.55	Joback Method
cpg	1089.25	J/mol×K	1012.33	Joback Method
cpg	1074.84	J/mol×K	977.12	Joback Method
cpg	1136.45	J/mol×K	1153.20	Joback Method
dvisc	0.0000304	Pa×s	941.90	Joback Method

dvisc	0.0000392	Pa×s	881.43	Joback Method
dvisc	0.0000525	Pa×s	820.96	Joback Method
dvisc	0.0000738	Pa×s	760.49	Joback Method
dvisc	0.0001098	Pa×s	700.02	Joback Method
dvisc	0.0001761	Pa×s	639.55	Joback Method
dvisc	0.0003118	Pa×s	579.08	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U381314&Units=SI

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