

Succinic acid, 8-bromooctyl 8-chlorooctyl ester

Inchi:	InChI=1S/C20H36BrClO4/c21-15-9-5-1-3-7-11-17-25-19(23)13-14-20(24)26-18-12-8-4-2
InchiKey:	LSLDNIIIIVVTCRQ-UHFFFAOYSA-N
Formula:	C20H36BrClO4
SMILES:	O=C(CCC(=O)OCCCCCCCCBr)OCCCCCCCCCl
Mol. weight [g/mol]:	455.85

Physical Properties

Property code	Value	Unit	Source
gf	-347.93	kJ/mol	Joback Method
hf	-935.14	kJ/mol	Joback Method
hfus	62.61	kJ/mol	Joback Method
hvap	89.25	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	6.168		Crippen Method
mcvol	337.280	ml/mol	McGowan Method
pc	1100.81	kPa	Joback Method
rinpol	3039.00		NIST Webbook
tb	913.17	K	Joback Method
tc	1118.08	K	Joback Method
tf	549.20	K	Joback Method
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1045.17	J/molxK	913.17	Joback Method
cpg	1113.86	J/molxK	1083.93	Joback Method
cpg	1102.29	J/molxK	1049.78	Joback Method
cpg	1089.66	J/molxK	1015.63	Joback Method
cpg	1075.96	J/molxK	981.47	Joback Method
cpg	1061.14	J/molxK	947.32	Joback Method
cpg	1124.43	J/molxK	1118.08	Joback Method
dvisc	0.0000344	Paxs	913.17	Joback Method
dvisc	0.0000448	Paxs	852.51	Joback Method

dvisc	0.0000607	Paxs	791.85	Joback Method
dvisc	0.0000866	Paxs	731.18	Joback Method
dvisc	0.0001316	Paxs	670.52	Joback Method
dvisc	0.0002175	Paxs	609.86	Joback Method
dvisc	0.0004016	Paxs	549.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381315&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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