

Succinic acid, 7-bromoheptyl 7-chloroheptyl ester

Inchi:	InChI=1S/C18H32BrClO4/c19-13-7-3-1-5-9-15-23-17(21)11-12-18(22)24-16-10-6-2-4-8-1
InchiKey:	FFZKFXKSCIBBAE-UHFFFAOYSA-N
Formula:	C18H32BrClO4
SMILES:	O=C(CCC(=O)OCCCCCBr)OCCCCCCCCI
Mol. weight [g/mol]:	427.80

Physical Properties

Property code	Value	Unit	Source
gf	-364.77	kJ/mol	Joback Method
hf	-893.86	kJ/mol	Joback Method
hfus	57.43	kJ/mol	Joback Method
hvap	84.79	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	5.388		Crippen Method
mvol	309.100	ml/mol	McGowan Method
pc	1255.70	kPa	Joback Method
rinpol	2862.00		NIST Webbook
tb	867.41	K	Joback Method
tc	1064.80	K	Joback Method
tf	526.66	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	925.26	J/molxK	867.41	Joback Method
cpg	991.27	J/molxK	1031.90	Joback Method
cpg	979.99	J/molxK	999.00	Joback Method
cpg	967.78	J/molxK	966.10	Joback Method
cpg	954.60	J/molxK	933.21	Joback Method
cpg	940.43	J/molxK	900.31	Joback Method
cpg	1001.63	J/molxK	1064.80	Joback Method
dvisc	0.0000470	Paxs	867.41	Joback Method
dvisc	0.0000609	Paxs	810.62	Joback Method

dvisc	0.0000820	Paxs	753.83	Joback Method
dvisc	0.0001158	Paxs	697.04	Joback Method
dvisc	0.0001740	Paxs	640.24	Joback Method
dvisc	0.0002830	Paxs	583.45	Joback Method
dvisc	0.0005110	Paxs	526.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382409&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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