

Succinic acid, 8-bromooctyl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C19H35BrO4/c1-4-11-17(16(2)3)24-19(22)13-12-18(21)23-15-10-8-6-5-7-9-14
InchiKey:	WKMOBKFKDJEOOG-UHFFFAOYSA-N
Formula:	C19H35BrO4
SMILES:	CCCC(OC(=O)CCC(=O)OCCCCCCCCBr)C(C)C
Mol. weight [g/mol]:	407.38

Physical Properties

Property code	Value	Unit	Source
gf	-349.30	kJ/mol	Joback Method
hf	-909.32	kJ/mol	Joback Method
hfus	48.78	kJ/mol	Joback Method
hvap	81.86	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	5.413		Crippen Method
mcvol	310.950	ml/mol	McGowan Method
pc	1218.29	kPa	Joback Method
rinsol	2501.00		NIST Webbook
tb	851.98	K	Joback Method
tc	1047.33	K	Joback Method
tf	478.01	K	Joback Method
vc	1.198	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.72	J/molxK	851.98	Joback Method
cpg	974.33	J/molxK	884.54	Joback Method
cpg	989.87	J/molxK	917.10	Joback Method
cpg	1004.36	J/molxK	949.66	Joback Method
cpg	1017.82	J/molxK	982.21	Joback Method
cpg	1030.27	J/molxK	1014.77	Joback Method
cpg	1041.74	J/molxK	1047.33	Joback Method
dvisc	0.0007569	Paxs	478.01	Joback Method
dvisc	0.0003500	Paxs	540.34	Joback Method

dvisc	0.0001898	Paxs	602.67	Joback Method
dvisc	0.0001155	Paxs	665.00	Joback Method
dvisc	0.0000765	Paxs	727.32	Joback Method
dvisc	0.0000541	Paxs	789.65	Joback Method
dvisc	0.0000402	Paxs	851.98	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=U381313&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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