

Succinic acid, ethyl 7-bromoheptyl ester

Inchi:	InChI=1S/C13H23BrO4/c1-2-17-12(15)8-9-13(16)18-11-7-5-3-4-6-10-14/h2-11H2,1H3
InchiKey:	IOBBYMVEMCHVPC-UHFFFAOYSA-N
Formula:	C13H23BrO4
SMILES:	CCOC(=O)CCC(=O)OCCCCCBr
Mol. weight [g/mol]:	323.22

Physical Properties

Property code	Value	Unit	Source
gf	-394.94	kJ/mol	Joback Method
hf	-774.92	kJ/mol	Joback Method
hfus	40.28	kJ/mol	Joback Method
hvap	69.28	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.218		Crippen Method
mvol	226.410	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
rinpol	2052.00		NIST Webbook
rinpol	2052.00		NIST Webbook
tb	715.58	K	Joback Method
tc	903.15	K	Joback Method
tf	440.39	K	Joback Method
vc	0.874	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.89	J/molxK	715.58	Joback Method
cpg	626.96	J/molxK	746.84	Joback Method
cpg	640.29	J/molxK	778.10	Joback Method
cpg	652.87	J/molxK	809.37	Joback Method
cpg	664.73	J/molxK	840.63	Joback Method
cpg	675.86	J/molxK	871.89	Joback Method
cpg	686.27	J/molxK	903.15	Joback Method
dvisc	0.0010712	Paxs	440.39	Joback Method

dvisc	0.0006196	Paxs	486.25	Joback Method
dvisc	0.0003939	Paxs	532.12	Joback Method
dvisc	0.0002690	Paxs	577.99	Joback Method
dvisc	0.0001944	Paxs	623.85	Joback Method
dvisc	0.0001468	Paxs	669.71	Joback Method
dvisc	0.0001150	Paxs	715.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382403&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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