

Succinic acid, butyl pent-4-enyl ester

Inchi:	InChI=1S/C13H22O4/c1-3-5-7-11-17-13(15)9-8-12(14)16-10-6-4-2/h3H,1,4-11H2,2H3
InchiKey:	UUOYQQSCROZCGV-UHFFFAOYSA-N
Formula:	C13H22O4
SMILES:	C=CCCCOC(=O)CCC(=O)OCCCC
Mol. weight [g/mol]:	242.31

Physical Properties

Property code	Value	Unit	Source
gf	-321.42	kJ/mol	Joback Method
hf	-675.82	kJ/mol	Joback Method
hfus	33.72	kJ/mol	Joback Method
hvap	62.17	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.619		Crippen Method
mvol	204.610	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
rinpol	1643.00		NIST Webbook
rinpol	1643.00		NIST Webbook
tb	646.10	K	Joback Method
tc	824.98	K	Joback Method
tf	378.83	K	Joback Method
vc	0.792	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.83	J/molxK	646.10	Joback Method
cpg	560.42	J/molxK	675.91	Joback Method
cpg	574.33	J/molxK	705.73	Joback Method
cpg	587.56	J/molxK	735.54	Joback Method
cpg	600.14	J/molxK	765.35	Joback Method
cpg	612.06	J/molxK	795.17	Joback Method
cpg	623.32	J/molxK	824.98	Joback Method
dvisc	0.0015761	Paxs	378.83	Joback Method

dvisc	0.0008541	Paxs	423.38	Joback Method
dvisc	0.0005201	Paxs	467.92	Joback Method
dvisc	0.0003453	Paxs	512.46	Joback Method
dvisc	0.0002447	Paxs	557.01	Joback Method
dvisc	0.0001825	Paxs	601.55	Joback Method
dvisc	0.0001417	Paxs	646.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353370&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
mccvol:	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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