

Sebacic acid, di(but-3-enyl) ester

Inchi: InChI=1S/C18H30O4/c1-3-5-15-21-17(19)13-11-9-7-8-10-12-14-18(20)22-16-6-4-2/h3-4H
InchiKey: OJYNZEKRFKIIRG-UHFFFAOYSA-N
Formula: C18H30O4
SMILES: C=CCCOC(=O)CCCCCCCCC(=O)OCCC=C
Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	-191.48	kJ/mol	Joback Method
hf	-653.59	kJ/mol	Joback Method
hfus	45.39	kJ/mol	Joback Method
hvap	72.63	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.346		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
pc	1303.29	kPa	Joback Method
rinpol	2178.00		NIST Webbook
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tb	757.18	K	Joback Method
tc	937.96	K	Joback Method
tf	433.42	K	Joback Method
vc	1.054	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.03	J/molxK	757.18	Joback Method
cpg	814.39	J/molxK	787.31	Joback Method
cpg	829.87	J/molxK	817.44	Joback Method
cpg	844.49	J/molxK	847.57	Joback Method
cpg	858.27	J/molxK	877.70	Joback Method
cpg	871.23	J/molxK	907.83	Joback Method
cpg	883.39	J/molxK	937.96	Joback Method
dvisc	0.0010483	Paxs	433.42	Joback Method

dvisc	0.0005380	Paxs	487.38	Joback Method
dvisc	0.0003154	Paxs	541.34	Joback Method
dvisc	0.0002037	Paxs	595.30	Joback Method
dvisc	0.0001414	Paxs	649.26	Joback Method
dvisc	0.0001039	Paxs	703.22	Joback Method
dvisc	0.0000797	Paxs	757.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356096&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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