

Sebacic acid, 3-methylbut-2-enyl propyl ester

Inchi:	InChI=1S/C18H32O4/c1-4-14-21-17(19)11-9-7-5-6-8-10-12-18(20)22-15-13-16(2)3/h13H
InchiKey:	XDRCCTVUZJZOLT-UHFFFAOYSA-N
Formula:	C18H32O4
SMILES:	CCCOC(=O)CCCCCCCCC(=O)OCC=C(C)C
Mol. weight [g/mol]:	312.44

Physical Properties

Property code	Value	Unit	Source
gf	-295.49	kJ/mol	Joback Method
hf	-797.02	kJ/mol	Joback Method
hfus	46.84	kJ/mol	Joback Method
hvap	74.01	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.570		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1278.25	kPa	Joback Method
rinpol	2201.00		NIST Webbook
tb	767.86	K	Joback Method
tc	951.28	K	Joback Method
tf	417.90	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.84	J/molxK	767.86	Joback Method
cpg	841.82	J/molxK	798.43	Joback Method
cpg	857.90	J/molxK	829.00	Joback Method
cpg	873.09	J/molxK	859.57	Joback Method
cpg	887.43	J/molxK	890.14	Joback Method
cpg	900.92	J/molxK	920.71	Joback Method
cpg	913.59	J/molxK	951.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355875&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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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