

Sebacic acid, butyl heptyl ester

Inchi:	InChI=1S/C21H40O4/c1-3-5-7-12-15-19-25-21(23)17-14-11-9-8-10-13-16-20(22)24-18-6
InchiKey:	XIIZQLGCKWEZDF-UHFFFAOYSA-N
Formula:	C21H40O4
SMILES:	CCCCCCCCOC(=O)CCCCCCCC(=O)OCCCC
Mol. weight [g/mol]:	356.54

Physical Properties

Property code	Value	Unit	Source
gf	-341.90	kJ/mol	Joback Method
hf	-966.37	kJ/mol	Joback Method
hfus	55.72	kJ/mol	Joback Method
hvap	80.65	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.964		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1012.95	kPa	Joback Method
rinqol	2524.00		NIST Webbook
tb	832.46	K	Joback Method
tc	1019.85	K	Joback Method
tf	470.75	K	Joback Method
vc	1.260	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.26	J/molxK	832.46	Joback Method
cpg	1048.96	J/molxK	863.69	Joback Method
cpg	1066.54	J/molxK	894.92	Joback Method
cpg	1083.03	J/molxK	926.15	Joback Method
cpg	1098.44	J/molxK	957.39	Joback Method
cpg	1112.80	J/molxK	988.62	Joback Method
cpg	1126.13	J/molxK	1019.85	Joback Method
dvisc	0.0007511	Paxs	470.75	Joback Method
dvisc	0.0003622	Paxs	531.03	Joback Method

dvisc	0.0002027	Paxs	591.32	Joback Method
dvisc	0.0001263	Paxs	651.61	Joback Method
dvisc	0.0000852	Paxs	711.89	Joback Method
dvisc	0.0000612	Paxs	772.17	Joback Method
dvisc	0.0000461	Paxs	832.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354305&Units=SI

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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