Sebacic acid, butyl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C21H40O4/c1-6-7-16-24-19(22)14-12-10-8-9-11-13-15-20(23)25-21(17(2)3)18
InchiKey: NCTYGTKVCDTUKF-UHFFFAOYSA-N
Formula: C21H40O4
SMILES: CCCCOC(=O)CCCCCCCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]: 356.54

Physical Properties

Property code	Value	Unit	Source
gf	-349.22	kJ/mol	Joback Method
hf	-982.21	kJ/mol	Joback Method
hfus	45.15	kJ/mol	Joback Method
hvap	79.49	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.674		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1028.60	kPa	Joback Method
rinpol	2337.00		NIST Webbook
tb	831.14	K	Joback Method
tc	1020.11	K	Joback Method
tf	425.75	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.67	J/mol×K	831.14	Joback Method
cpg	1114.48	J/mol×K	988.62	Joback Method
cpg	1100.16	J/mol×K	957.12	Joback Method
cpg	1084.74	J/mol×K	925.63	Joback Method
cpg	1068.19	J/mol×K	894.13	Joback Method
cpg	1050.51	J/mol×K	862.64	Joback Method
cpg	1127.72	J/mol×K	1020.11	Joback Method
dvisc	0.0000355	Pa×s	831.14	Joback Method
dvisc	0.0000496	Pa×s	763.58	Joback Method

dvisc	0.0000739	Pa×s	696.01	Joback Method
dvisc	0.0001201	Pa×s	628.44	Joback Method
dvisc	0.0002191	Pa×s	560.88	Joback Method
dvisc	0.0004714	Pa×s	493.32	Joback Method
dvisc	0.0012935	Pa×s	425.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355426&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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