Sebacic acid, butyl 4-formylphenyl ester

Inchi: InChI=1S/C21H30O5/c1-2-3-16-25-20(23)10-8-6-4-5-7-9-11-21(24)26-19-14-12-18(17-22
InchiKey: QKOUCWXVAUQWLG-UHFFFAOYSA-N
Formula: C21H30O5
SMILES: CCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C=O)cc1
Mol. weight [g/mol]: 362.46

Physical Properties

Property code	Value	Unit	Source
gf	-338.64	kJ/mol	Joback Method
hf	-826.89	kJ/mol	Joback Method
hfus	51.66	kJ/mol	Joback Method
hvap	90.31	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	4.869		Crippen Method
mcvol	299.440	ml/mol	McGowan Method
pc	1320.39	kPa	Joback Method
rinpol	2901.00		NIST Webbook
rinpol	2901.00		NIST Webbook
tb	912.78	K	Joback Method
tc	1121.15	K	Joback Method
tf	551.69	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	952.82	J/mol×K	912.78	Joback Method
cpg	967.35	J/mol×K	947.51	Joback Method
cpg	980.65	J/mol×K	982.24	Joback Method
cpg	992.76	J/mol×K	1016.97	Joback Method
cpg	1003.71	J/mol×K	1051.70	Joback Method
cpg	1013.53	J/mol×K	1086.42	Joback Method
cpg	1022.23	J/mol×K	1121.15	Joback Method
dvisc	0.0005069	Pa×s	551.69	Joback Method

dvisc	0.0002865	Pa×s	611.87	Joback Method
dvisc	0.0001794	Pa×s	672.05	Joback Method
dvisc	0.0001213	Pa×s	732.23	Joback Method
dvisc	0.0000871	Pa×s	792.42	Joback Method
dvisc	0.0000655	Pa×s	852.60	Joback Method
dvisc	0.0000511	Pa×s	912.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354887&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

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