Sebacic acid, butyl 3-iodobenzyl ester

Inchi: InChI=1S/C21H31IO4/c1-2-3-15-25-20(23)13-8-6-4-5-7-9-14-21(24)26-17-18-11-10-12-1
InchiKey: FZTIUEQRFBADNO-UHFFFAOYSA-N
Formula: C21H31IO4
SMILES: CCCCOC(=O)CCCCCCCCC(=O)OCc1cccc(I)c1
Mol. weight [g/mol]: 474.37

Physical Properties

Property code	Value	Unit	Source
gf	-181.00	kJ/mol	Joback Method
hf	-664.44	kJ/mol	Joback Method
hfus	53.78	kJ/mol	Joback Method
hvap	92.96	kJ/mol	Joback Method
log10ws	-7.08		Crippen Method
logp	5.798		Crippen Method
mcvol	323.690	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rinpol	2973.00		NIST Webbook
rinpol	2973.00		NIST Webbook
tb	957.26	K	Joback Method
tc	1177.82	K	Joback Method
tf	567.75	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.07	J/mol×K	957.26	Joback Method
cpg	1003.20	J/mol×K	994.02	Joback Method
cpg	1016.10	J/mol×K	1030.78	Joback Method
cpg	1027.83	J/mol×K	1067.54	Joback Method
cpg	1038.42	J/mol×K	1104.30	Joback Method
cpg	1047.92	J/mol×K	1141.06	Joback Method
cpg	1056.38	J/mol×K	1177.82	Joback Method
dvisc	0.0003687	Pa×s	567.75	Joback Method

dvisc	0.0002008	Pa×s	632.67	Joback Method
dvisc	0.0001225	Pa×s	697.59	Joback Method
dvisc	0.0000813	Pa×s	762.50	Joback Method
dvisc	0.0000575	Pa×s	827.42	Joback Method
dvisc	0.0000428	Pa×s	892.34	Joback Method
dvisc	0.0000331	Pa×s	957.26	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380754&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