

Sebacic acid, butyl 2-iodobenzyl ester

Inchi:	InChI=1S/C21H31IO4/c1-2-3-16-25-20(23)14-8-6-4-5-7-9-15-21(24)26-17-18-12-10-11-1
InchiKey:	JPZWCVPVIFISLSQL-UHFFFAOYSA-N
Formula:	C21H31IO4
SMILES:	CCCCOC(=O)CCCCCCCCC(=O)OCc1ccccc1I
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	2972.00		NIST Webbook
rinpol	2972.00		NIST Webbook
tb	957.26	K	Joback Method
tc	1177.82	K	Joback Method
tf	567.75	K	Joback Method
vc	1.240	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002008	Paxs	632.67	Joback Method
dvisc	0.0001225	Paxs	697.59	Joback Method
dvisc	0.0000813	Paxs	762.50	Joback Method
dvisc	0.0000575	Paxs	827.42	Joback Method
dvisc	0.0000428	Paxs	892.34	Joback Method
dvisc	0.0000331	Paxs	957.26	Joback Method

Sources

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=U380671&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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