

Sebacic acid, 4-iodobenzyl isobutyl ester

Inchi: InChI=1S/C21H31IO4/c1-17(2)15-25-20(23)9-7-5-3-4-6-8-10-21(24)26-16-18-11-13-19(2)
InchiKey: PIPKGYHXEJVYIX-UHFFFAOYSA-N
Formula: C21H31IO4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OCc1ccc(I)cc1
Mol. weight [g/mol]: 474.37

Physical Properties

Property code	Value	Unit	Source
gf	-183.44	kJ/mol	Joback Method
hf	-669.72	kJ/mol	Joback Method
hfus	50.26	kJ/mol	Joback Method
hvap	92.57	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	5.654		Crippen Method
mcvol	323.690	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
rinpola	2955.00		NIST Webbook
rinpola	2955.00		NIST Webbook
tb	956.82	K	Joback Method
tc	1178.71	K	Joback Method
tf	552.75	K	Joback Method
vc	1.234	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.51	J/molxK	956.82	Joback Method
cpg	1048.25	J/molxK	1141.73	Joback Method
cpg	1038.82	J/molxK	1104.75	Joback Method
cpg	1028.28	J/molxK	1067.77	Joback Method
cpg	1016.58	J/molxK	1030.78	Joback Method
cpg	1003.67	J/molxK	993.80	Joback Method
cpg	1056.60	J/molxK	1178.71	Joback Method
dvisc	0.0000302	Paxs	956.82	Joback Method

dvisc	0.0000395	Paxs	889.47	Joback Method
dvisc	0.0000540	Paxs	822.13	Joback Method
dvisc	0.0000782	Paxs	754.78	Joback Method
dvisc	0.0001215	Paxs	687.44	Joback Method
dvisc	0.0002079	Paxs	620.10	Joback Method
dvisc	0.0004055	Paxs	552.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380624&Units=SI
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

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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