Sebacic acid, 4-iodobenzyl nonyl ester

Inchi: InChI=1S/C26H41IO4/c1-2-3-4-5-8-11-14-21-30-25(28)15-12-9-6-7-10-13-16-26(29)31-2
InchiKey: WFDVPVXGFLVIDI-UHFFFAOYSA-N
Formula: C26H41IO4
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1ccc(I)cc1
Mol. weight [g/mol]: 544.51

Physical Properties

Property code	Value	Unit	Source
gf	-138.90	kJ/mol	Joback Method
hf	-767.64	kJ/mol	Joback Method
hfus	66.73	kJ/mol	Joback Method
hvap	104.09	kJ/mol	Joback Method
log10ws	-9.18		Crippen Method
logp	7.749		Crippen Method
mcvol	394.140	ml/mol	McGowan Method
pc	902.89	kPa	Joback Method
rinpol	3495.00		NIST Webbook
rinpol	3495.00		NIST Webbook
tb	1071.66	K	Joback Method
tc	1313.53	K	Joback Method
tf	624.10	K	Joback Method
vc	1.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1294.41	J/mol×K	1071.66	Joback Method
cpg	1309.62	J/mol×K	1111.97	Joback Method
cpg	1323.28	J/mol×K	1152.28	Joback Method
cpg	1335.50	J/mol×K	1192.59	Joback Method
cpg	1346.34	J/mol×K	1232.91	Joback Method
cpg	1355.89	J/mol×K	1273.22	Joback Method
cpg	1364.24	J/mol×K	1313.53	Joback Method
dvisc	0.0001949	Pa×s	624.10	Joback Method

dvisc	0.0001012	Pa×s	698.69	Joback Method
dvisc	0.0000596	Pa×s	773.29	Joback Method
dvisc	0.0000385	Pa×s	847.88	Joback Method
dvisc	0.0000267	Pa×s	922.47	Joback Method
dvisc	0.0000196	Pa×s	997.07	Joback Method
dvisc	0.0000150	Pa×s	1071.66	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=U380631&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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