Sebacic acid, heptyl 3-iodobenzyl ester

Inchi: InChI=1S/C24H37IO4/c1-2-3-4-9-12-18-28-23(26)16-10-7-5-6-8-11-17-24(27)29-20-21-1
InchiKey: UALBYCYVYDXNOS-UHFFFAOYSA-N
Formula: C24H37IO4
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)OCc1cccc(I)c1
Mol. weight [g/mol]: 516.45

Physical Properties

Property code	Value	Unit	Source
gf	-155.74	kJ/mol	Joback Method
hf	-726.36	kJ/mol	Joback Method
hfus	61.55	kJ/mol	Joback Method
hvap	99.64	kJ/mol	Joback Method
log10ws	-8.34		Crippen Method
logp	6.969		Crippen Method
mcvol	365.960	ml/mol	McGowan Method
pc	1016.83	kPa	Joback Method
rinpol	3186.00		NIST Webbook
rinpol	3186.00		NIST Webbook
tb	1025.90	K	Joback Method
tc	1256.07	K	Joback Method
tf	601.56	K	Joback Method
vc	1.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1170.90	J/mol×K	1025.90	Joback Method
cpg	1185.60	J/mol×K	1064.26	Joback Method
cpg	1198.92	J/mol×K	1102.62	Joback Method
cpg	1210.92	J/mol×K	1140.98	Joback Method
cpg	1221.67	J/mol×K	1179.34	Joback Method
cpg	1231.22	J/mol×K	1217.71	Joback Method
cpg	1239.64	J/mol×K	1256.07	Joback Method
dvisc	0.0002534	Pa×s	601.56	Joback Method

dvisc	0.0001340	Pa×s	672.28	Joback Method
dvisc	0.0000800	Pa×s	743.01	Joback Method
dvisc	0.0000522	Pa×s	813.73	Joback Method
dvisc	0.0000365	Pa×s	884.45	Joback Method
dvisc	0.0000269	Pa×s	955.18	Joback Method
dvisc	0.0000207	Pa×s	1025.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380757&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