Isophthalic acid, 6-ethyloct-3-yl isobutyl ester

Inchi: InChI=1S/C22H34O4/c1-6-17(7-2)12-13-20(8-3)26-22(24)19-11-9-10-18(14-19)21(23)25
InchiKey: ZZBOJSXLHFXCSA-UHFFFAOYSA-N
Formula: C22H34O4
SMILES: CCC(CC)CCC(CC)OC(=O)c1cccc(C(=O)OCC(C)C)c1
Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-238.02	kJ/mol	Joback Method
hf	-777.79	kJ/mol	Joback Method
hfus	41.39	kJ/mol	Joback Method
hvap	84.65	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	5.651		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1190.70	kPa	Joback Method
rinpol	2500.00		NIST Webbook
rinpol	2500.00		NIST Webbook
tb	885.68	K	Joback Method
tc	1092.54	K	Joback Method
tf	475.96	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.73	J/mol×K	885.68	Joback Method
cpg	1015.52	J/mol×K	920.16	Joback Method
cpg	1031.00	J/mol×K	954.63	Joback Method
cpg	1045.19	J/mol×K	989.11	Joback Method
cpg	1058.14	J/mol×K	1023.59	Joback Method
cpg	1069.87	J/mol×K	1058.07	Joback Method
cpg	1080.41	J/mol×K	1092.54	Joback Method
dvisc	0.0007173	Pa×s	475.96	Joback Method

dvisc	0.0003074	Pa×s	544.25	Joback Method
dvisc	0.0001592	Pa×s	612.53	Joback Method
dvisc	0.0000940	Pa×s	680.82	Joback Method
dvisc	0.0000611	Pa×s	749.11	Joback Method
dvisc	0.0000427	Pa×s	817.39	Joback Method
dvisc	0.0000315	Pa×s	885.68	Joback Method

Sources

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=U344678&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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