

Isophthalic acid, 1-propylbutyl tridecyl ester

Inchi: InChI=1S/C28H46O4/c1-4-7-8-9-10-11-12-13-14-15-16-22-31-27(29)24-20-17-21-25(23-26)
InchiKey: HUGLGLWDPGLUQW-UHFFFAOYSA-N
Formula: C28H46O4
SMILES: CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(CCC)CCC)c1
Mol. weight [g/mol]: 446.66

Physical Properties

Property code	Value	Unit	Source
gf	-182.62	kJ/mol	Joback Method
hf	-891.07	kJ/mol	Joback Method
hfus	63.98	kJ/mol	Joback Method
hvap	98.78	kJ/mol	Joback Method
log10ws	-9.60		Crippen Method
logp	8.280		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	821.01	kPa	Joback Method
rinpol	3099.00		NIST Webbook
tb	1023.84	K	Joback Method
tc	1257.25	K	Joback Method
tf	573.58	K	Joback Method
vc	1.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1369.87	J/molxK	1023.84	Joback Method
cpg	1443.15	J/molxK	1218.35	Joback Method
cpg	1431.78	J/molxK	1179.45	Joback Method
cpg	1418.83	J/molxK	1140.55	Joback Method
cpg	1404.24	J/molxK	1101.64	Joback Method
cpg	1387.95	J/molxK	1062.74	Joback Method
cpg	1453.02	J/molxK	1257.25	Joback Method
dvisc	0.0000152	Paxs	1023.84	Joback Method
dvisc	0.0000203	Paxs	948.80	Joback Method

dvisc	0.0000283	Paxs	873.75	Joback Method
dvisc	0.0000422	Paxs	798.71	Joback Method
dvisc	0.0000682	Paxs	723.67	Joback Method
dvisc	0.0001234	Paxs	648.62	Joback Method
dvisc	0.0002604	Paxs	573.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356408&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

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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