

Terephthalic acid, but-3-enyl undecyl ester

Inchi: InChI=1S/C23H34O4/c1-3-5-7-8-9-10-11-12-13-19-27-23(25)21-16-14-20(15-17-21)22(2
InchiKey: YBSGXKOBWLZQZ-UHFFFAOYSA-N
Formula: C23H34O4
SMILES: C=CCCOC(=O)c1ccc(C(=O)OCCCCCCCCCCC)cc1
Mol. weight [g/mol]: 374.51

Physical Properties

Property code	Value	Unit	Source
gf	-134.44	kJ/mol	Joback Method
hf	-657.16	kJ/mol	Joback Method
hfus	53.27	kJ/mol	Joback Method
hvap	87.37	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	6.107		Crippen Method
mvol	321.750	ml/mol	McGowan Method
pc	1129.10	kPa	Joback Method
rinpol	2859.00		NIST Webbook
tb	906.56	K	Joback Method
tc	1112.82	K	Joback Method
tf	530.47	K	Joback Method
vc	1.244	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1029.39	J/molxK	906.56	Joback Method
cpg	1045.71	J/molxK	940.94	Joback Method
cpg	1060.79	J/molxK	975.31	Joback Method
cpg	1074.68	J/molxK	1009.69	Joback Method
cpg	1087.40	J/molxK	1044.06	Joback Method
cpg	1098.99	J/molxK	1078.44	Joback Method
cpg	1109.50	J/molxK	1112.82	Joback Method
dvisc	0.0004436	Paxs	530.47	Joback Method
dvisc	0.0002378	Paxs	593.15	Joback Method

dvisc	0.0001436	Paxs	655.83	Joback Method
dvisc	0.0000947	Paxs	718.52	Joback Method
dvisc	0.0000668	Paxs	781.20	Joback Method
dvisc	0.0000496	Paxs	843.88	Joback Method
dvisc	0.0000384	Paxs	906.56	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=U356341&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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