

Terephthalic acid, isobutyl 2-methylpent-3-yl ester

Inchi:	InChI=1S/C18H26O4/c1-6-16(13(4)5)22-18(20)15-9-7-14(8-10-15)17(19)21-11-12(2)3/h
InchiKey:	PEZKWXLHNSOVPS-UHFFFAOYSA-N
Formula:	C18H26O4
SMILES:	CCC(OC(=O)c1ccc(C(=O)OCC(C)C)cc1)C(C)C
Mol. weight [g/mol]:	306.40

Physical Properties

Property code	Value	Unit	Source
gf	-271.70	kJ/mol	Joback Method
hf	-695.23	kJ/mol	Joback Method
hfus	31.03	kJ/mol	Joback Method
hvap	75.75	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.091		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1582.23	kPa	Joback Method
rinpol	2091.00		NIST Webbook
rinpol	2091.00		NIST Webbook
tb	794.16	K	Joback Method
tc	1001.35	K	Joback Method
tf	430.88	K	Joback Method
vc	0.966	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.86	J/molxK	794.16	Joback Method
cpg	832.78	J/molxK	966.82	Joback Method
cpg	821.04	J/molxK	932.29	Joback Method
cpg	808.19	J/molxK	897.75	Joback Method
cpg	794.22	J/molxK	863.22	Joback Method
cpg	779.12	J/molxK	828.69	Joback Method
cpg	843.45	J/molxK	1001.35	Joback Method
dvisc	0.0000559	Paxs	794.16	Joback Method

dvisc	0.0000751	Paxs	733.61	Joback Method
dvisc	0.0001063	Paxs	673.07	Joback Method
dvisc	0.0001612	Paxs	612.52	Joback Method
dvisc	0.0002680	Paxs	551.97	Joback Method
dvisc	0.0005049	Paxs	491.43	Joback Method
dvisc	0.0011366	Paxs	430.88	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=U356193&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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