

Terephthalic acid, isobutyl 2-heptyl ester

Inchi:	InChI=1S/C19H28O4/c1-5-6-7-8-15(4)23-19(21)17-11-9-16(10-12-17)18(20)22-13-14(2)3
InchiKey:	VTKGLNMUXPDPAY-UHFFFAOYSA-N
Formula:	C19H28O4
SMILES:	CCCCC(C)OC(=O)c1ccc(C(=O)OCC(C)C)cc1
Mol. weight [g/mol]:	320.42

Physical Properties

Property code	Value	Unit	Source
gf	-260.84	kJ/mol	Joback Method
hf	-710.59	kJ/mol	Joback Method
hfus	37.15	kJ/mol	Joback Method
hvap	78.36	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.625		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1459.02	kPa	Joback Method
rinqol	2225.00		NIST Webbook
tb	817.48	K	Joback Method
tc	1021.25	K	Joback Method
tf	457.15	K	Joback Method
vc	1.028	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.12	J/molxK	817.48	Joback Method
cpg	836.35	J/molxK	851.44	Joback Method
cpg	851.44	J/molxK	885.40	Joback Method
cpg	865.39	J/molxK	919.36	Joback Method
cpg	878.23	J/molxK	953.32	Joback Method
cpg	889.98	J/molxK	987.28	Joback Method
cpg	900.66	J/molxK	1021.25	Joback Method
dvisc	0.0008629	Paxs	457.15	Joback Method
dvisc	0.0004138	Paxs	517.21	Joback Method

dvisc	0.0002312	Paxs	577.26	Joback Method
dvisc	0.0001441	Paxs	637.32	Joback Method
dvisc	0.0000975	Paxs	697.37	Joback Method
dvisc	0.0000702	Paxs	757.42	Joback Method
dvisc	0.0000530	Paxs	817.48	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=U356287&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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