Dibut-3-enyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, dibut-3-enyl ester
Dibut-3-enyl-1,2-benzenedicarboxylate
Inchi: InChI=1S/C16H18O4/c1-3-5-11-19-15(17)13-9-7-8-10-14(13)16(18)20-12-6-4-2/h3-4,7-1
InchiKey: PHSVKLDVWSRDNM-UHFFFAOYSA-N
Formula: C16H18O4
SMILES: C=CCCOC(=O)c1ccccc1C(=O)OCCC=C
Mol. weight [g/mol]: 274.31

Physical Properties

Property code	Value	Unit	Source
gf	-105.54	kJ/mol	Joback Method
hf	-387.25	kJ/mol	Joback Method
hfus	33.86	kJ/mol	Joback Method
hvap	71.12	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.152		Crippen Method
mcvol	218.820	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	1939.00		NIST Webbook
rinpol	1939.00		NIST Webbook
tb	743.08	K	Joback Method
tc	950.66	K	Joback Method
tf	449.82	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.61	J/mol×K	743.08	Joback Method
cpg	612.64	J/mol×K	777.68	Joback Method
cpg	625.73	J/mol×K	812.27	Joback Method
cpg	637.90	J/mol×K	846.87	Joback Method
cpg	649.17	J/mol×K	881.46	Joback Method
cpg	659.55	J/mol×K	916.06	Joback Method

cpg	669.08	J/mol×K	950.66	Joback Method
dvisc	0.0008637	Pa×s	449.82	Joback Method
dvisc	0.0005114	Pa×s	498.70	Joback Method
dvisc	0.0003325	Pa×s	547.57	Joback Method
dvisc	0.0002320	Pa×s	596.45	Joback Method
dvisc	0.0001709	Pa×s	645.33	Joback Method
dvisc	0.0001315	Pa×s	694.20	Joback Method
dvisc	0.0001047	Pa×s	743.08	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=U373496&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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