

3-Butyl-oxirane-2-carboxylic acid methyl ester

Inchi:	InChI=1S/C8H14O3/c1-3-4-5-6-7(11-6)8(9)10-2/h6-7H,3-5H2,1-2H3
InchiKey:	PWCHCSPGSPYCEF-UHFFFAOYSA-N
Formula:	C8H14O3
SMILES:	CCCCC1OC1C(=O)OC
Mol. weight [g/mol]:	158.19

Physical Properties

Property code	Value	Unit	Source
gf	-250.52	kJ/mol	Joback Method
hf	-532.79	kJ/mol	Joback Method
hfus	26.45	kJ/mol	Joback Method
hvap	46.67	kJ/mol	Joback Method
log10ws	-1.24		Crippen Method
logp	1.117		Crippen Method
mcvol	126.030	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	1083.00		NIST Webbook
tb	487.75	K	Joback Method
tc	675.95	K	Joback Method
tf	292.35	K	Joback Method
vc	0.484	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.45	J/molxK	487.75	Joback Method
cpg	308.66	J/molxK	519.12	Joback Method
cpg	321.28	J/molxK	550.48	Joback Method
cpg	333.31	J/molxK	581.85	Joback Method
cpg	344.78	J/molxK	613.22	Joback Method
cpg	355.69	J/molxK	644.59	Joback Method
cpg	366.07	J/molxK	675.95	Joback Method
dvisc	0.0018407	Paxs	292.35	Joback Method
dvisc	0.0013542	Paxs	324.92	Joback Method

dvisc	0.0010535	Paxs	357.48	Joback Method
dvisc	0.0008547	Paxs	390.05	Joback Method
dvisc	0.0007162	Paxs	422.62	Joback Method
dvisc	0.0006154	Paxs	455.18	Joback Method
dvisc	0.0005397	Paxs	487.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R249266&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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