

Butyl 2,4-dichlorobenzoate

Inchi:	InChI=1S/C11H12Cl2O2/c1-2-3-6-15-11(14)9-5-4-8(12)7-10(9)13/h4-5,7H,2-3,6H2,1H3
InchiKey:	VEUZBKXIJHGTFT-UHFFFAOYSA-N
Formula:	C11H12Cl2O2
SMILES:	CCCCOC(=O)c1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	247.12

Physical Properties

Property code	Value	Unit	Source
gf	-122.89	kJ/mol	Joback Method
hf	-333.06	kJ/mol	Joback Method
hfus	28.69	kJ/mol	Joback Method
hvap	61.61	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.950		Crippen Method
mvol	174.010	ml/mol	McGowan Method
pc	2497.50	kPa	Joback Method
rinpol	1695.00		NIST Webbook
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tb	638.87	K	Joback Method
tc	857.81	K	Joback Method
tf	397.19	K	Joback Method
vc	0.665	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.95	J/molxK	638.87	Joback Method
cpg	409.15	J/molxK	675.36	Joback Method
cpg	420.60	J/molxK	711.85	Joback Method
cpg	431.31	J/molxK	748.34	Joback Method
cpg	441.31	J/molxK	784.83	Joback Method
cpg	450.59	J/molxK	821.32	Joback Method
cpg	459.17	J/molxK	857.81	Joback Method
dvisc	0.0011863	Paxs	397.19	Joback Method

dvisc	0.0007483	Paxs	437.47	Joback Method
dvisc	0.0005101	Paxs	477.75	Joback Method
dvisc	0.0003691	Paxs	518.03	Joback Method
dvisc	0.0002798	Paxs	558.31	Joback Method
dvisc	0.0002202	Paxs	598.59	Joback Method
dvisc	0.0001786	Paxs	638.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373008&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	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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