

butyl cis-4-heptenoate

Inchi:	InChI=1S/C11H20O2/c1-3-5-7-8-9-11(12)13-10-6-4-2/h5,7H,3-4,6,8-10H2,1-2H3/b7-5-
InchiKey:	QAYIJRHHNQPAOG-ALCCZGGFSA-N
Formula:	C11H20O2
SMILES:	CCC=CCCC(=O)OCCCC
Mol. weight [g/mol]:	184.28

Physical Properties

Property code	Value	Unit	Source
gf	-111.96	kJ/mol	Joback Method
hf	-397.95	kJ/mol	Joback Method
hfus	27.24	kJ/mol	Joback Method
hvap	49.19	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.076		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
ripol	1564.00		NIST Webbook
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tb	531.53	K	Joback Method
tc	709.61	K	Joback Method
tf	280.81	K	Joback Method
vc	0.655	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.35	J/molxK	531.53	Joback Method
cpg	464.33	J/molxK	679.93	Joback Method
cpg	452.12	J/molxK	650.25	Joback Method
cpg	439.33	J/molxK	620.57	Joback Method
cpg	425.95	J/molxK	590.89	Joback Method
cpg	411.96	J/molxK	561.21	Joback Method
cpg	475.98	J/molxK	709.61	Joback Method
dvisc	0.0001740	Paxs	531.53	Joback Method

dvisc	0.0002282	Paxs	489.74	Joback Method
dvisc	0.0003149	Paxs	447.96	Joback Method
dvisc	0.0004643	Paxs	406.17	Joback Method
dvisc	0.0007484	Paxs	364.38	Joback Method
dvisc	0.0013650	Paxs	322.60	Joback Method
dvisc	0.0029775	Paxs	280.81	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=R493408&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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