2-Butoxyethyl 3,5,5-trimethylhexanoate

Inchi: InChI=1S/C15H30O3/c1-6-7-8-17-9-10-18-14(16)11-13(2)12-15(3,4)5/h13H,6-12H2,1-5H
InchiKey: FKSRCXOXNDMDDE-UHFFFAOYSA-N
Formula: C15H30O3
SMILES: CCCCOCCOC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]: 258.40

Physical Properties

Property code	Value	Unit	Source
gf	-263.10	kJ/mol	Joback Method
hf	-743.98	kJ/mol	Joback Method
hfus	27.64	kJ/mol	Joback Method
hvap	58.87	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.809		Crippen Method
mcvol	235.520	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
rinpol	1603.00		NIST Webbook
rinpol	1603.00		NIST Webbook
tb	637.64	K	Joback Method
tc	814.79	K	Joback Method
tf	340.62	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.85	J/mol×K	637.64	Joback Method
cpg	735.84	J/mol×K	785.27	Joback Method
cpg	721.07	J/mol×K	755.74	Joback Method
cpg	705.50	J/mol×K	726.22	Joback Method
cpg	689.12	J/mol×K	696.69	Joback Method
cpg	671.91	J/mol×K	667.17	Joback Method
cpg	749.85	J/mol×K	814.79	Joback Method
dvisc	0.0000864	Pa×s	637.64	Joback Method

dvisc	0.0001201	Pa×s	588.14	Joback Method
dvisc	0.0001773	Pa×s	538.63	Joback Method
dvisc	0.0002831	Pa×s	489.13	Joback Method
dvisc	0.0005024	Pa×s	439.63	Joback Method
dvisc	0.0010314	Pa×s	390.12	Joback Method
dvisc	0.0026093	Pa×s	340.62	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378248&Units=SI

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