

Glutaric acid, butyl 7-bromoheptyl ester

Inchi:	InChI=1S/C16H29BrO4/c1-2-3-13-20-15(18)10-9-11-16(19)21-14-8-6-4-5-7-12-17/h2-14
InchiKey:	RQQAYDFABWDVDI-UHFFFAOYSA-N
Formula:	C16H29BrO4
SMILES:	CCCCOC(=O)CCCC(=O)OCCCCCBr
Mol. weight [g/mol]:	365.30

Physical Properties

Property code	Value	Unit	Source
gf	-369.68	kJ/mol	Joback Method
hf	-836.84	kJ/mol	Joback Method
hfus	48.05	kJ/mol	Joback Method
hvap	75.96	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.389		Crippen Method
mvol	268.680	ml/mol	McGowan Method
pc	1487.29	kPa	Joback Method
rinpol	2345.00		NIST Webbook
rinpol	2345.00		NIST Webbook
tb	784.22	K	Joback Method
tc	971.96	K	Joback Method
tf	474.20	K	Joback Method
vc	1.042	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.43	J/molxK	784.22	Joback Method
cpg	795.78	J/molxK	815.51	Joback Method
cpg	810.24	J/molxK	846.80	Joback Method
cpg	823.84	J/molxK	878.09	Joback Method
cpg	836.60	J/molxK	909.38	Joback Method
cpg	848.52	J/molxK	940.67	Joback Method
cpg	859.62	J/molxK	971.96	Joback Method
dvisc	0.0007993	Paxs	474.20	Joback Method

dvisc	0.0004439	Paxs	525.87	Joback Method
dvisc	0.0002739	Paxs	577.54	Joback Method
dvisc	0.0001829	Paxs	629.21	Joback Method
dvisc	0.0001299	Paxs	680.88	Joback Method
dvisc	0.0000968	Paxs	732.55	Joback Method
dvisc	0.0000750	Paxs	784.22	Joback Method

Sources

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=U380502&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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