Glutaric acid, 2-(3-bromophenyl)ethyl heptyl ester

Inchi: InChI=1S/C20H29BrO4/c1-2-3-4-5-6-14-24-19(22)11-8-12-20(23)25-15-13-17-9-7-10-18(

InchiKey: QNTPOEPXDUXOCQ-UHFFFAOYSA-N

Formula: C20H29BrO4

SMILES: CCCCCCCOC(=O)CCCC(=O)OCCc1cccc(Br)c1

Mol. weight [g/mol]: 413.35

Physical Properties

Property code	Value	Unit	Source
gf	-233.22	kJ/mol	Joback Method
hf	-694.34	kJ/mol	Joback Method
hfus	52.07	kJ/mol	Joback Method
hvap	87.80	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.219		Crippen Method
mcvol	301.280	ml/mol	McGowan Method
pc	1412.25	kPa	Joback Method
rinpol	2811.00		NIST Webbook
rinpol	2811.00		NIST Webbook
tb	907.40	K	Joback Method
tc	1118.87	K	Joback Method
tf	558.22	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.16	J/mol×K	907.40	Joback Method
cpg	932.61	J/mol×K	942.64	Joback Method
cpg	945.91	J/mol×K	977.89	Joback Method
cpg	958.11	J/mol×K	1013.13	Joback Method
cpg	969.22	J/mol×K	1048.38	Joback Method
cpg	979.30	J/mol×K	1083.62	Joback Method
cpg	988.36	J/mol×K	1118.87	Joback Method
dvisc	0.0003888	Pa×s	558.22	Joback Method

dvisc	0.0002264	Pa×s	616.42	Joback Method
dvisc	0.0001448	Pa×s	674.61	Joback Method
dvisc	0.0000994	Pa×s	732.81	Joback Method
dvisc	0.0000721	Pa×s	791.01	Joback Method
dvisc	0.0000546	Pa×s	849.20	Joback Method
dvisc	0.0000429	Pa×s	907.40	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=U377210&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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